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SERVICES FOR RESEARCH INTO THE REACTIVITY OF MUSTARD IN MIXED SOLVENT

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SRI has carefully measured the rate of hydrolysis of mustard in mixed EtOH/water over a range of mole fractions from X = 0.025 to X = 0.075 and a temperature range of 11°C to 45°C. The rate constants at 25°C and X = 0.025 are k_1 = 1.20 x [illegible] and k_2 = 6.7 x 10^{-3} sec^{-1}. The activation parameters, which are calculated from the temperature dependence of the rate constant at X = 0.025 using the Arrhenius expression, are Ea_{k_1} = 22.59 Kcal/mol, lnA = 31.91 for k_1 and Ea_{k_2} = 17.90 Kcal/mol, lnA = 15.49 for k_2.

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PREFACE

The work described in this report was authorized under Contract No. DAAK11-84-C-0008. This work was started in January 1984 and completed in January 1985.

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This report has been approved for release to the public.

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INTRODUCTION

Background.

On the night of July 12, 1917, the Germans used artillery shells loaded with mustard gas against the British front near Ypres during the Battle of Flanders.[1] In the intervening years, mustard has proven to be a very effective military agent and is still a threat.[2] The persistency of mustard is a particular problem--more than half a century after the Battle of Flanders residents of Ypres were still being burned by mustard residues.[3]

Many researchers have studied the chemistry of mustard and have concluded that although it is subject to oxidation by strong oxidizing agents, the primary chemical reaction is hydrolysis.[3-11] Mustard (HD) readily undergoes pH-independent hydrolysis by the complex mechanism shown in Figure 1.[3-15] In the intramolecular case, involving only mustard or mustard chlorohydrin and solvent, hydrolysis proceeds through episulfonium ions II and IV, leading first to mustard chlorohydrin and then to thiodiglycol [Reactions (2) and (4)]. An equivalent of hydrogen ion and chloride ion are produced in each step. Bartlett and Swain[4] showed that these reactions are independent of pH in the range 6 to 10, although mustard is dehydrochlorinated in a base-sensitive elimination at high pH to yield vinylsulfides.[5,8,16]

In general, intermolecular self- reactions of mustard and its products accompany hydrolysis; these reactions result in sulfonium ions VI, VII, and VIII. However, at low starting concentrations of mustard, these reactions are negligible.

Stein, Moore, and Bergmann[5] report that sulfonium ion formation accounts for at least 16% of the starting mass of HD at a starting volume ratio of 0.005 HD/H_2O and 5% at a volume ratio of 0.001 HD/H_2O. Bartlett and Swain[4] found that 2.2% dimeric product was formed in experiments that kept the initial mustard concentration below 0.001 M, which corresponds to volume ratio of about 1×10^{-4}.

Low concentrations of mustard also slow the recapture of chloride ion through the back reactions of (1) and (2) in Figure 1 because large concentrations of Cl^- are never produced. Barllett and Swain[4] showed that added chloride ion up to 0.0019 M did not significantly affect the rate of hydrolysis of mustard or mustard chlorohydrin, but that a ten-fold increase in chloride ion to 0.019 M resulted in a 25% diminution of each rate.

Reactions (1) and (2) are rate-limiting. Under these conditions, Bartlett and Swain demonstrated that both hydrogen ion and chloride ion are liberated according to the biexponential equation

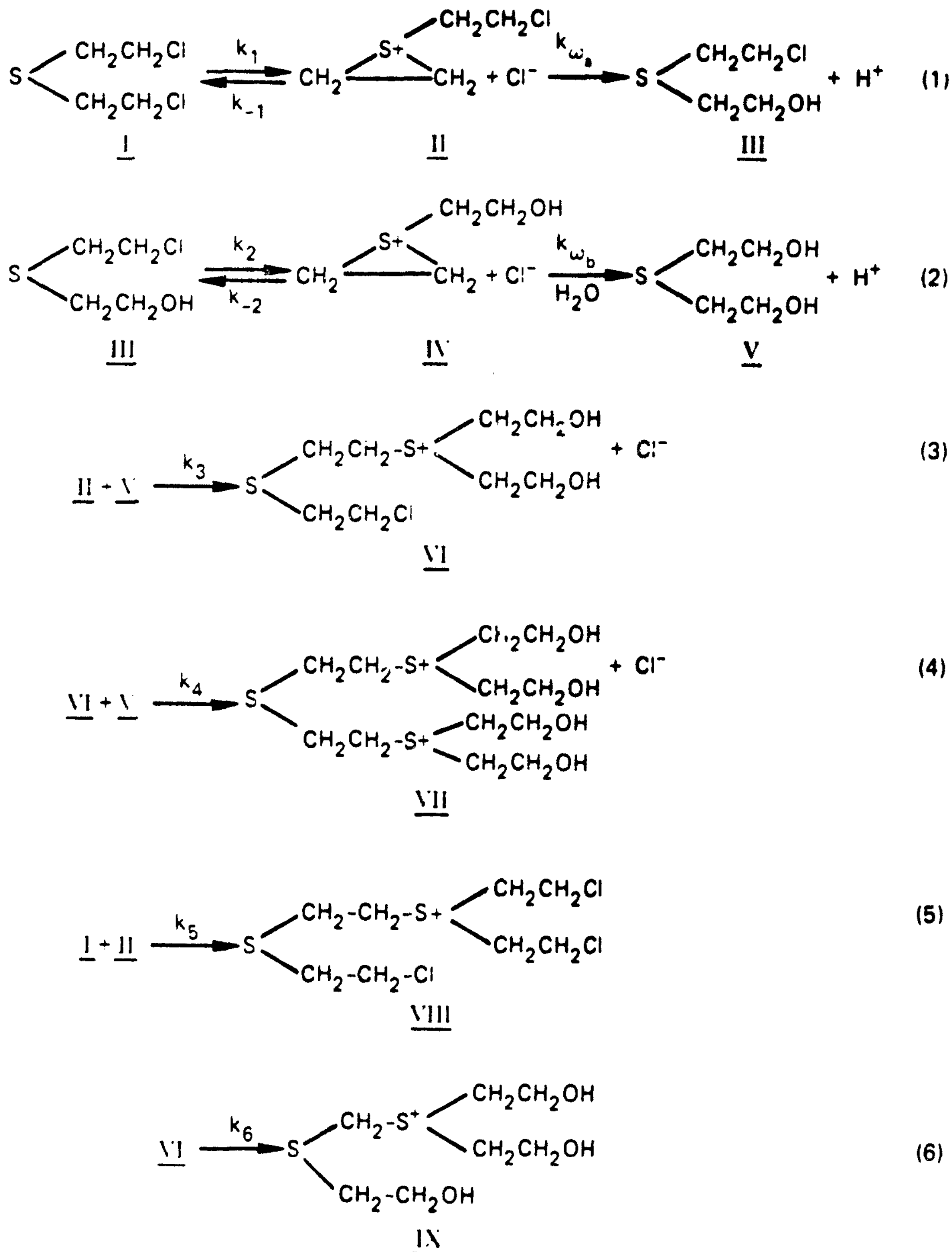

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Figure 1. Transformation and Hydrolysis of Mustard.

$$[H^+] = [Cl^-] = [HD]_o\left[2 - \left(\frac{k_1 - 2k_3}{k_1 - k_3}\right)e^{-k_1 t} - \left(\frac{k_1}{k_1 - k_3}\right)e^{-k_3 t}\right] \qquad (7)$$

in which $[HD]_o$ is the initial concentration of mustard. This is the integrated rate equation for a sequence of two, consecutive, unimolecular reactions specifically applied to the mechanism shown in Figure 1. Bartlett and Swain[4] were able to determine k_1 by independently measuring k_2 and best-fitting $[H^+]$ data with equation (7); this was done by changing k_1 using a graphical technique developed by Swain.[17]

A number of problems exist with the use of Bartlett and Swain's results for calculation of decontamination rates and environmental lifetimes. First, the study was conducted in a mixed solvent system at only one composition, and thus the sensitivity to solvent has not been determined. Second, the study was conducted at only one temperature so that the activation energies are unknown. Third, the second rate constant k_2 was not determined in the experiment, but was measured by synthesizing the intermediate (chlorohydrin) and analyzing its hydrolysis rate. Finally, the rate constants were determined by a graphical technique rather than by least squares computer fit.

The two most crucial problems are the lack of an activation energy and the use of a mixed solvent system rather than water. A number of other early sources have measured the rate in pure water at several different temperatures.[6,18-21] However the rate constants determined by these investigators were based on the assumption that the reaction could be fit to a first-order expression. Thus, the activation energies may be incorrect.

J. R. Ward and R. P. Seiders[12,14] have evaluated the kinetic data for mustard hydrolysis from many of these sources[4,18-21] They redetermined the rate constants from the raw data by using modern computational techniques and fitting the data to consecutive first-order reactions. They found that only Bartlett and Swain's data fitted satisfactorily to the consecutive first-order expression. Thus, Ward and Seiders concluded that some systematic experimental error caused deviations from consecutive first-order reactions and that the activation parameters from these studies are not reliable.

Objectives.

The current study was conceived to fill the void in the data for mustard hydrolysis. Our objectives were to measure the hydrolysis of mustard at several different temperatures and determine reliable activation parameters. A supplementary goal was to determine the source of the systematic experimental error present in the earlier studies, so that such errors can be avoided. In addition, we attempted to determine the effect of mixed solvents on the hydrolysis rate. The rate constants k_1 and k_2 were both to be determined from the data through the use of modern computational techniques. SRI's success in accomplishing these goals is reported herein.

EXPERIMENTAL DETAILS

Materials.

Mustard (HD) was supplied by U.S. Army CRDC and used as received. The purity of the material, as determined by gas chromatography, was 99.5%. No significant decomposition was evident over the time period of these experiments. Millipore water was degassed by N_2 purge before use. Absolute ethanol was used as obtained from U.S Industrial Chemical Corporation. Nitrogen was supplied from liquid carbonic. Sodium hydroxide and perchloric acid were supplied by Baker. Chloroethyl ethyl sulfide was supplied by Aldrich Chemical.

Apparatus.

All kinetic evaluations were conducted on the multiple computer-controlled pH stat; and the User's Guide for this pH stat control program is reproduced in Appendix C. The pH stat was built to maintain constant pH in the reaction solution and to have the three characteristics discussed below, which we were unable to find in commercial pH stats.

The first requirement is that the pH stat must record the observed changes in pH and the amount of acid or base added as a function of time. For an acid- or base-producing reaction (such as the hydrolysis of mustard discussed here), the amount of added titrant is a measure of reaction progress at that time. These data should be handled by a computer requiring that the pH stat be computer interfaced. Ideally the computer can also be used to calculate rate constants and related kinetic parameters directly from the data.

The second requirement is the ability to control several experiments simultaneously, thereby increasing the number of experiments conducted within a given time period. Thus, instruments that can control only one experiment can be a bottleneck for efficient experimental work.

The third requirement is that the pH stat should be highly flexible with respect to operating parameters. For example, a small or large volume of titrant should be added to the controlled solution in response to a small or large deviation from the desired pH.

Figure 2 illustrates the overall configuration of the system that we have assembled to meet these criteria.

The central element in the system is the computer, in our case a Digital Equipment Corporation MINC-11/2. The computer is currently equipped with a terminal, a printer, and a floppy disc system for mass data storage, and a modem for mass data transfer. Also being used are a real time-clock, an analog-to-digital converter, and four digital output modules.

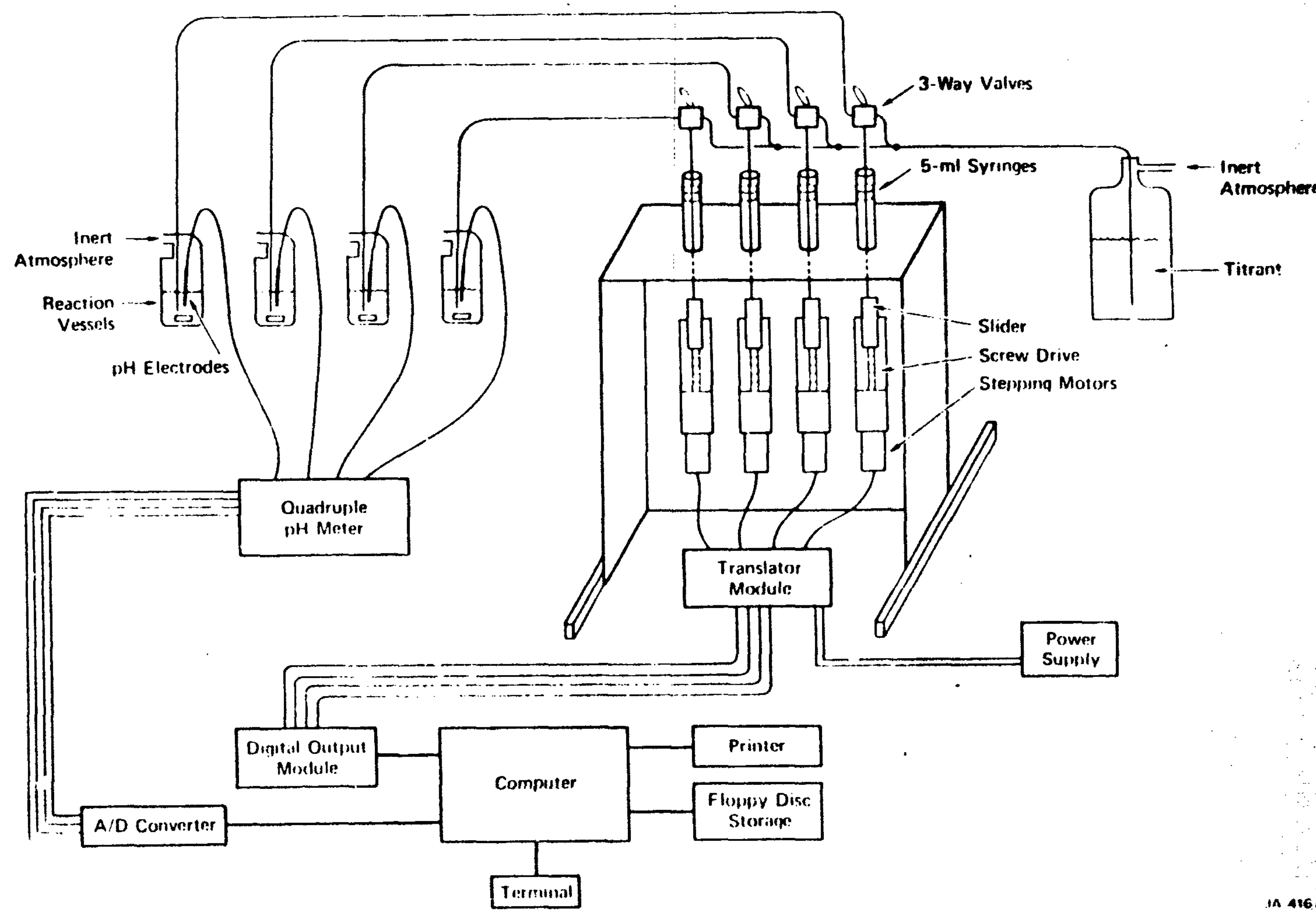

Figure 2. Quadruple pH Stat.

The analog-to-digital converter is used to convert the signal for digital input to the computer; a similar device is used in a traditional digital pH meter. The analog-to-digital converter receives four analog signals from the "quadruple pH meter." The quadruple pH meter consists of a power supply and four amplifiers. Each amplifiers consist of two stages. The first is an operational amplifier operating with near-unity gain. The electrode potential is applied to the noninverting input, and the variable gain resistor serves as the "slope" control. The second stage provides additional gain and a summing point to which a variable "offset" potential is applied. The two amplifiers are contained in a dual package RCA 3240 MOS/FET op-amp with 10^3 meg Ω input impedance.

Electrode potentials proportional to pH are generated from "Ross" combination pH electrodes (Orion Research Model 8102) with pH resolution of 0.002 units. The four electrodes are inserted into four reaction vessels, such as that shown in Figure 3. Each reaction vessel is water-jacketed to maintain temperature and is equipped with magnetic stirring bar, titrant inlet, and gas inlet/outlet. The temperature is maintained by circulating coolant (water/ethylene glycol) through the water jacket from a constant temperature bath. The titrant is introduced through Teflon tubes. A set of Teflon three-way valves allows each syringe to be filled from the titrant supply (which is also maintained under an inert atmosphere) if the valve is set in one position and the second valve position, allows the syringe to dispense titrant to the reaction vessel.

The syringes are Precision Sampling 5.0 ml gas-tight models with Teflon plungers and "special" Teflon connectors that couple with flanged Teflon tubing. Thus, the titrant is exposed only to glass and Teflon. The syringes are mounted vertically on the top of a box so that air bubbles can be expelled.

Mounted on the inside back of the box are four syringe pump drivers that consist of screw-driven sliding stages. The syringe pump drivers are connected by push rods to the syringe plungers. The screw driver units are operated by four stepping motors. (The assemblies are Velmex, Inc., Unislides, B2506CJ, with Superior Electric Slo-Syn Model M062-FD-04 stepping motors.) The drive screws advance the slider stages 0.025 inches per revolution, and the stepper motors have 200 steps per revolution. The syringe travel path is 2.36 inches. The total number of steps is 18,900 for 5.0 ml or one step for 0.265 μl. This minimum volume increment is about one fourth that of available pH stats. The maximum speed of titrant delivery is 0.75 ml/min.

The stepping motors are controlled by Superior Electric Slo-Syn ST101 translator modules and powered by a Power/Mate Corp. ES-24 G power supply rated at 24 V and 8 A. The translator modules are controlled by TTL compatible digital pulses from the digital output module of the MINC-11/2 computer.

We have reproduced an edited representative data file in Table 1 for a reaction maintained at pH = 4 that produces base. The data file shows the time, pH, number of 0.25 μℓ units of titrant that were added (which are called

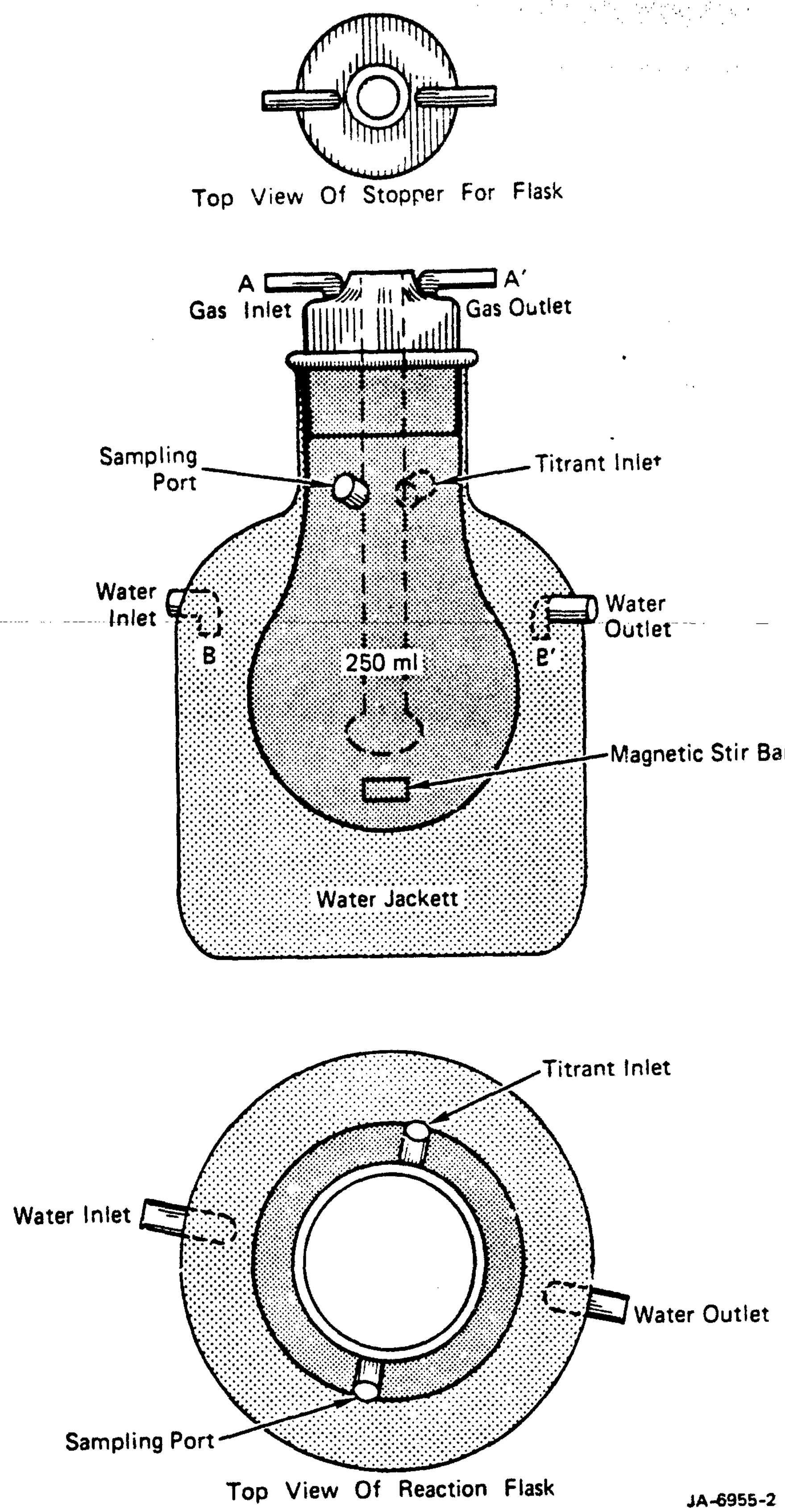

Figure 3. Reaction Vessel.

Table 1

Data File Produced by pH-Stat

	NBI Acid Titrant Stat No. 1		
Time	pH	Squirts	Cum-Sqrt
6.1650E+01	3.907	0	0
1.2483E+02	3.900	0	0
1.8800E+02	3.946	0	0
2.5267E+02	3.991	94	94
3.1667E+02	3.994	86	180
4.7611E+02	4.028	610	1095
5.5741E+02	4.003	614	1709
6.6296E+02	3.972	1426	3184
7.3992E+02	4.030	204	3338
8.3700E+02	4.086	979	4317
9.2925E+02	4.013	792	5109
1.0857E+03	4.080	1902	7011
1.1110E+03	4.080	162	7173
1.2070E+03	4.007	867	3040
1.2822E+03	4.005	306	3346

squirts), and the cumulative number of squirts. The data files are stored on floppy disk and can be printed directly using the printer associated with the MINC Computer.

An alternative data handling system has been developed as shown in Figure 4. We can transfer the data by modem from the pH Stat Control Program on the MINC laboratory computer to SRI's VAX 11/780 mainframe computer using a translation program called NET. Once the data are on the VAX, they can be manipulated as desired. In particular, we can use the data as input for kinetics programs.

Kinetic Procedures.

A typical kinetic study of mustard hydrolysis proceeded as follows. First 4 µl of neat mustard (5.08×10^{-3} g, 3.19×10^{-5} mole) is added to 4 ml of absolute ethanol by syringe. Then 2 ml of the ethanol solution of HD (2.54×10^{-3} g, 1.595×10^{-5} mole) is transferred to a 250-ml reaction vessel containing 17.25 ml of absolute EtOH and 230.7 ml of degassed millipore water; this is adjusted to pH 7. This resulted in a solution of 0.025 mole fraction EtOH. The hydrolysis is followed by starting the SRI pH-Stat in a recording mode. In this mode the pH stat records pH as a time function but does not add titrant. The pH-Stat is started simultaneously with injection of the HD. The remaining 2 ml of HD solution is then added to a second cell monitored by the pH-Stat. Because the pH-Stat has already started collecting data, a time delay is introduced in the second data set. This time delay is subsequently subtracted from the data set. The temperature is maintained in both cells by circulating coolant (water/ethylene glycol) through both cells from a constant temperature bath. We found that during these rapid reactions, the temperature in the cell was maintained ± 0.01°C. In all reactions conducted, the headspace at the reaction flask was purged with nitrogen.

Experiments were also conducted that varied from this procedure. In one set of experiments at 25°C the HD concentration was twice that reported above. The mole fraction of EtOh was varied (0.25, 0.50, and 0.75) at 25°C. In addition, one set of experiments was conducted using acetone as the cosolvent rather than ethanol.

The hydrolysis of chloroethyl ethylsulfide was conducted in a similar manner with 5% acetone as the solvent.

Kinetic Calculations.

The kinetic expression for consecutive irreversible first-order reactions was first derived by Esson in the early 1800s (as reported by Moore and Pearson).[22] Using the nomenclature shown in Figure 1, the reaction is

$$\begin{array}{l} \underline{I} \xrightarrow{k_1} \underline{III} + HCl \\ \qquad\quad \underline{III} \xrightarrow{k_2} V + HCl \end{array} \qquad (8)$$

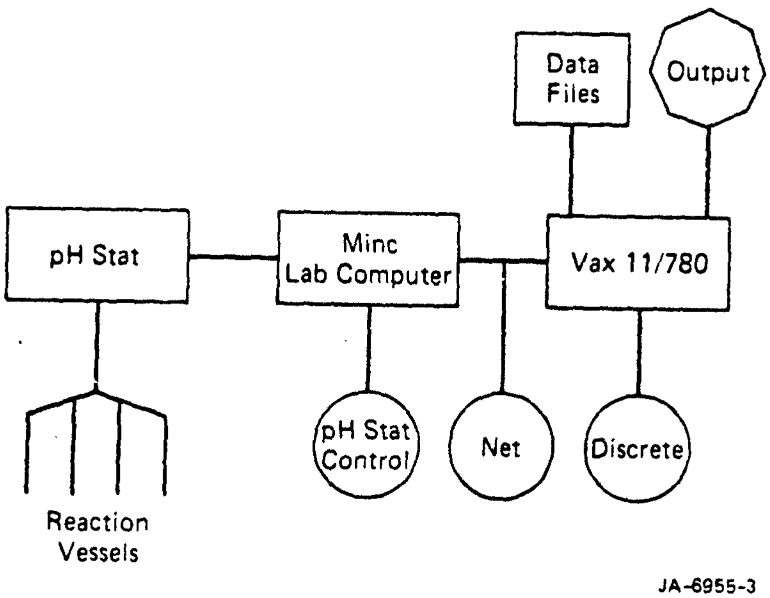

Figure 4. SRI Data Handling Scheme.

The differential equations for the reaction as written in (8) are

$$\frac{d(I)}{dt} = -k_1[I] \tag{9}$$

$$\frac{d(III)}{dt} = k_1[I] - k_2[III] \tag{10}$$

$$\frac{d(V)}{dt} = k_2[III] \tag{11}$$

$$\frac{d(HCl)}{dt} = k_1[I] + k_2[III] \tag{12}$$

The integrated form of equation (9) is

$$[I] = [I]_o^{\,e-k_1t} \tag{13}$$

Then substituting (13) into (10) gives

$$\frac{d(III)}{dt} = k_1[I]\ ^{ek_1t} - k_2[III] \qquad k_1[I]e^{-k_1t}\ k_2[III] \tag{14}$$

integration gives (if $[III]_o = 0$)

$$[III] = \frac{[I]_o k_1}{k_2 - k_1}\left(e^{-k_1t} - e^{-k_2t}\right) \tag{15}$$

Then from the stoichiometry of reaction (8) it is clear that

$$[II] = [I]_o - [I] - [III] \tag{16}$$

and substituting gives

$$[V] = [I]_o - [I]_o e^{-k_1t} - \frac{[I]_o k_1}{k_2 - k_1}\left(e^{-k_1t} - e^{-k_2t}\right) \tag{17}$$

Also from reaction (8) it is clear that

$$[HCl] = [III] + 2[V] \tag{18}$$

Substituting gives

$$[HCl] = \left(\frac{[I]_o k_1}{k_2 - k_1} e^{-k_1 t}\right) - e^{-k_2 t} + 2[I]_o - 2[I]_o e^{-k_1 t} - \frac{2[I]_o k_1}{k_1 - k_2}\left(e^{-k_1 t} - e^{-k_2 t}\right) \quad (19)$$

then (19) simplifies to (20)

$$[HCl] = [I]_o \left\{ 2 + \left(\frac{k_1 - 2k_2}{k_2 - k_1}\right) e^{-k_1 t} + \left(\frac{k_1}{k_2 - k_1}\right) e^{-k_2 t} \right\} \quad (20)$$

and transposition gives the more commonly seen form (21)

$$[HCl] = [I]_o \left\{ 2 - \left(\frac{k_1 - 2k_2}{k_1 - k_2}\right) e^{-k_1 t} - \left(\frac{k_1}{k_1 - k_2}\right) e^{-k_2 t} \right\}. \quad (21)$$

The rate constants k_1 and k_2 are determined from pH versus time data using an unbiased nonlinear least-squares method developed by Stephen Provencher.[23] The Provencher program, DISCRETE, performs a grid search of kinetic data to find the amplitudes and rate constants of an exponential series as in equation (22).

$$[H^+] = A_o + A_1 e^{-k_1 t} + A_2 e^{-k_2 t} \ldots. \quad (22)$$

The program uses a nonlinear F test to decide how many exponentials best fit the data.[23] The starting point for the grid search is determined by finding peaks in the Fourier transform of the data.

This method of solving for the rate constants provides a number of internal checks on the validity of the solutions other than the statistical checks which the fitting routine provides such as goodness of fit. The first internal check is that the program determines the best fit as that having the appropriate number of exponentials--in this case, two. Because A_o is a variable that is fit, the fit initial concentrations can be checked versus the experimental value since:

$$A_o = 2[I]_o \tag{23}$$

The other amplitude factors can also be used as internal checks because they are fit independently of k_1 and k_2; however, according to equation (21), they equal:

$$A_1 = -[I]_o\left(\frac{k_1 - 2k_2}{k_1 - k_2}\right) \tag{24}$$

and

$$A_2 = -[I]_o\left(\frac{k_1}{k_1 \quad k_2}\right) \tag{25}$$

The temperature dependence of the rate constants, k_1 and k_2, may be expressed in terms of the Arrhenius equation:

$$\ln k = \ln A - (E_a/R)T \tag{26}$$

or in a three-parameter equation

$$\ln k = A/T + B \ln T + C \tag{27}$$

Equation (27) more accurately correlates the temperature dependence for the pH-independent hydrolysis of alkyl halides.[24] These activation parameters (A, B, and C) can be used to calculate the activation entropy, enthalpy, and heat capacity as discussed by Hyne and Robertson:[24]

$$\Delta H^{\ddagger} = -R(2.303A - BT) \tag{28}$$

$$\Delta S^{\ddagger} = 2.303R(C + B \log T) + RB \tag{29}$$

$$\Delta Cp^{\ddagger} = RB \tag{30}$$

RESULTS

The data for hydrolysis of mustard at various temperatures are given in the figures and tables of Appendices A and B, respectively. The data for hydrolysis of mustard at eight temperatures between 11°C and 45°C are plotted in Figures A-1 through A-8 and tabulated in Tables B-1 through B-8. The duplicate data (second cell, see experimental) are also given. All these experiments were conducted in EtOH/water with a mole fraction of 0.025 and an initial mustard concentration of 6.4×10^{-5} M.

Data for mustard hydrolysis at three mole fractions of the mixed solvent system were collected at 25°C and 6.4×10^{-5} M initial mustard concentration The data for 0.025 x EtOH/water are shown in Figure A-4 and tabulated in Tables B-4. Tables B-9 and B-10 present the data for 0.050 and 0.075 mole fraction, and these are plotted in Figures A-9 and A-10, respectively.

The last three experiments were conducted as checks on the accuracy of our experimental method. First the Bartlett and Swain experiment[4] was reproduced as accurately as possible. Plotted in Figure A-11 is the data for mustard hydrolysis at 25°C in 5% acetone/water (V/V) at an initial mustard concentration of 6.4×10^{-5} M (see also Table B-11). The hydrolysis in 0.025 x EtOH/water at 25°C was repeated at twice the initial mole fraction, and these data can be found in Table B-12 and plotted in Figure A-12. Finally, the rate of response of the electrodes was checked by measuring the response time to added HCl; these data can be found in Table B-13 and Figure A-13.

We have also studied the hydrolysis of chloroethyl ethyl sulfide (CEES) using this technique; these data are plotted in Figure A-14 and tabulated in Table B-14.

The raw data are fit to exponential series (equation 22) using the DISCRETE program developed by Provencher.[23] The results fit a two-exponential equation (however, see the discussion below). The results for the hydrolysis of mustard in 0.025 x EtOH/water at several temperatures (data from Tables 3-10 and 3A-10A) are summarized in Table 2.

The results of the DISCRETE fit for different mole fractions of EtOH in water are collected in Table 3. Table 4 gives the DISCRETE results for the reaction at twice the initial HD concentration and for the reaction in 5% acetone.

Table 2

First-Order Rate Constants (sec^{-1}) for Hydrolysis of Mustard in EtOH/Water Mixtures at X = 0.025[a]

Temp (K)	$k_1(10^3)$	$\Delta k_1(10^3)$	$k_2(10^3)$	$\Delta k_2(10^3)$	$A_o(10^5)$	$\Delta A_o(10^5)$[b]	$A_1(10^4)$[c]	$\Delta A_1(10^4)$	$A_2(10^5)$[d]	$\Delta A_2(10^5)$
318	18.4	0.1	93.2	10	14.7	0.01	-2.08	0.02	7.28	1.0
	18.0	0.4	91.8	20	17.7	0.04	-2.84	0.10	16.42	3.0
avg	18.2	0.25	92.5	15	16.2	0.02	-2.46	0.06	11.85	2.0
313	12.9	0.6	40	12	12.5	0.04	-1.9	0.2	6.0	1.3
	14.2	2.5	27	9.6	18.4	0.02	-4.2	2.3	2.3	2.3
avg	13.6	1.6	34	10.8	15.4	0.03	-3.0	1.2	4.2	1.8
308	10.1	0.9	16	3	13.2	0.02	-3.2	1.3	18	13
	8.3	0.2	25	2.3	16.4	0.03	-2.3	0.1	12	1.3
avg	9.2	0.6	20	2.6	14.8	0.02	-2.8	0.7	15	7
303	2.93	0.04	11.2	0.5	18.8	0.04	-2.98	0.05	12.1	0.5
	3.38	0.10	6.2	0.6	18.6	0.02	-3.02	0.31	11.6	3.1
avg	3.16	0.07	8.7	0.5	18.7	0.03	-3.00	0.18	11.8	1.8
298	1.82	0.02	7.0	0.4	9.2	0.07	-1.35	0.02	4.5	0.2
	1.58	0.03	6.4	0.4	8.7	0.02	-1.30	0.03	4.4	0.3
avg	1.70	0.02	6.7	0.4	9.0	0.04	-1.32	0.02	4.4	0.2
293	No fit									
288	0.544	0.004	4.1	0.3	6.4	0.01	-0.772	0.004	1.35	0.05
	1.031	0.013	—	—	8.6	3.30	-0.888	0.330	—	—
avg	0.288	0.008	4.1	0.3	7.5	1.66	-0.830	0.167	1.35	0.05
284	0.292	0.002	1.74	0.09	3.0	0.004	-0.265	0.002	0.59	0.02
	0.320	0.002	2.47	0.11	4.6	0.01	-0.550	0.002	0.90	0.02
avg	0.306	0.002	2.10	0.10	3.8	0.01	-0.458	0.002	0.74	0.02

[a] See Experimental Details section.

[b] $A_o = 2[HD]_o$.

[c] $A_1 = [HD]_o\left(\frac{k_1 - 2k_2}{k_1 - k_2}\right)$.

[d] $A_2 = -[HD]_o\left(\frac{k_1}{k_1 - k_2}\right)$.

[e] Δ are computer determinated standard deviations.

Table 3

First-Order Rate Constants (sec^{-1}) for Hydrolysis of Mustard in EtOH/Water Mixtures at 25°C[a]

X ethanol	$k_1(10^3)$	$\Delta k_1(10^3)$[e]	$k_2(10^3)$	$\Delta k_2(10^3)$	$A_o(10^5)$	$\Delta A_o(10^5)$[b]	$A_1(10^7)$[c]	$\Delta A_1(10^7$	$A_2(10^5)$[d]	$\Delta A_2(10^5)$
0.025	1.70	0.02	6.7	0.4	9.0	0.04	-1.32	0.02	4.4	0.2
0.050	1.70	0.04	8.2	0.6	9.3	0.04	-1.29	0.02	3.8	0.2
0.075	1.67	0.20	4.4	0.6	8.8	0.20	-1.81	0.30	9.9	2.7

[a] See Experimental Details section.

[b] $A_o = 2[HD]_o$.

[c] $A_1 = [HD]_o\left(\frac{k_1 - 2k_2}{k_1 - k_2}\right)$.

[d] $A_2 = -[HD]_o\left(\frac{k_1}{k_1 - k_2}\right)$.

[e] Δ are computer determinated standard deviations.

Table 4

First-Order Rate Constants (sec^{-1}) for Hydrolysis of Mustard at 25°C[a]

Condition	$k_1(10^3)$	$\Delta k_1(10^3)$[e]	$k_2(10^3)$	$\Delta k_2(10^3)$	$A_o(10^5)$	$\Delta A_o(10^5)$[b]	$A_1(10^4)$[c]	$\Delta A_1(10^5)$	$A_2(10^5)$[d]	$\Delta A_2(10^5)$
5% Acetone	2.44	0.30	5.8	2.0	10.2	0.1	-1.75	0.4	7.2	4.0
0.025 X EtOH/ 2 x $[HD]_o$	1.88	0.09	7.9	3.0	20.3	0.01	-2.45	0.1	3.7	1.0

[a]See Experimental Details section.

[b]$A_o = 2[HD]_o$.

[c]$A_1 = [HD]_o\left(\frac{k_1 - 2k_2}{k_1 - k_2}\right)$.

[d]$A_2 = [HD]_o\left(\frac{k_1}{k_1 - k_2}\right)$.

[e]Δ are computer determinated standard deviations.

DISCUSSION

The analysis of the data presented in the previous section requires that the following questions be answered. Are the data reliable? How good is the fit to the kinetics expression? How good is the computational technique used to fit the data to the kinetic expression? Is the experimental technique appropriate?

The activation parameters can be calculated from the results presented in Table 2. The reliability of the resulting activation parameters depends on the answers to the set of questions above. The activation parameters can be used to make some conclusions about the reaction mechanism.

The first criteria of useful reliable data for mustard hydrolysis using the DISCRETE program for data analysis is whether the program fits the data to a two-component expression. The data set presented in Table 2 is good by this criteria. The data from 45°C to 25°C (10 separate data sets) all fit the two-component criteria. Below 25°C, the data deviate somewhat. The 20°C data could not be fit by DISCRETE, the 15°C data were fit to a single exponential, and the 11°C data fit to a three-component fit; however, the two-component fit had equal probability and it is the two-component fit that is reported in Table 2. Thus, at two temperatures (20°C and 15°C) the data are not fit by DISCRETE to two components as required by the mechanism.

Ward and Seiders[14] have used the experimental fit of the initial mustard concentration as a diagnostic and appear to use an error of ± 50% as being within an appropriate range. The fit value of $[HD]_0$, which is $A_0/2$, is compared in Table 5 with the experimental value, and the percent deviation is calculated. All the deviations are less than 50% except for the 11°C data. Notice also in Table 5 that there is a systematic decrease in apparent $[HD]_0$ with lower temperatures, with the exception of the 30°C data. The source of this systematic variation of the fit value of $[HD]_0$ with temperature is not apparent. Because this value has been used as a criteria for the quality of the data, this variation is of concern and worthy of further study. One possible explanation can be seen in the plots shown in Appendix A, the initial slope of the plot is temperature dependent and correlates with the observed deviations for the calculated initial mustard concentration. Since the calculated $[HD]_0$ is essentially the y intercept, any initial rate deviations will effect the calculated $[HD]_0$ to a much greater extent. More calculations are needed to show conclusively that this explanation is correct. The source of the initial rate deviations and their temperature dependence is unclear and should be further investigated.

Table 5

Comparison of Calculated and Experimental $[HD]_o$[a]

Temp.(% C)	$[HD]_o$ (10^3 M)	% Deviation
Experimental	6.4	—
45	8.1	26
40	7.7	20
35	7.4	16
30	9.3	45
25	4.5	-30
20	—	—
15	3.8	-40
11	1.9	-70

[a]Based on the DISCRETE Fit of A_o, which is defined as $A_o = 2[HD]_o$.

The initial mustard concentrations calculated using A_1 and A_2 from the DISCRETE fit are shown in Table 6. These values do not agree as well with the experimental as the values shown in Table 5.

Table 6

Comparison of $[HD]_o$ Calculated from the DISCRETE Values for A_1[a] AND A_2[b]

Temp. (°C)	$[HD]_o$ (10^5 M)	% Dev.	$[HD]_o$ (10^5 M)[b]	% Dev.
Experimental	6.4	—	6.4	—
45	11	72	48	650
40	11	72	6.3	2
35	9.0	53	18	181
30	12	88	21	228
25	5.6	-12	13	103
20	—	—	—	—
15	2.7	-58	18	181
11	2.1	-67	4.3	-33

[a]Based on the DISCRETE fit for $A_1 = \frac{-[HD]_o(k_1-k_2)}{(k_1-2k_2)}$.

[b]Based on the DISCRETE fit for $A_2 = \frac{-[HD]_o(k_1-k_2)}{k_1}$.

A third method of checking the quality of the data is to compare the results of two runs that are identical except for the initial mustard concentration. The rate constant should be independent of initial mustard concentration at low concentrations. The results are shown in Table 4, where $k_1 = 1.88 \times 10^{-3}$ and $k_2 = 7.9 \times 10^{-3}$ (sec^{-1}) at 1.28×10^{-4} M mustard and 298 K. Table 2 shows $k_1 = 1.70 \times 10^{-3}$ and $k_2 = 6.7 \times 10^{-3}$ (sec^{-1}) at 6.4×10^{-5} M mustard and 298 K. These values are essentially identical. The range of two runs for k_1 from Table 2 is 1.82×10^{-3} to 1.58×10^{-3}; thus 1.88×10^{-3} is within 2 σ of the average 1.70×10^{-3}.)

Another check is to reproduce closely an experiment that is well accepted. In this case the data of Bartlett and Swain at 25°C in 5% acetone (V/V) are the best available.[4] We reproduced their experiment at 25°C and in 5% acetone (V/V). The only parameter that was different in our experiment was the initial mustard concentration; we used 6.4×10^{-5} M compared with 1×10^{-3} M for Bartlett and Swain. The resulting rate constants are compared in Table 7. The new data

Table 7

Comparison of Rate Constants Obtained by Different Calculation Routines

Data Set	Fitting Routine	k_1 (min^{-1})	k_2 (min^{-1})
Wilson and Burrows	DISCRETE	0.146 ± 0.02	0.35 ± 0.10
Bartlett and Swain	DISCRETE	0.137 ± 0.03	0.37 ± 0.04
Bartlett and Swain	Swain Graphical	0.155 ± 0.01	0.26 ± 0.03
Bartlett and Swain	CRDC nonlinear LSD	0.163 ± 0.01	0.22 ± 0.001

(Wilson and Burrows) are in good agreement with the data of Bartlett and Swain (difference is less than σ).

Table 7 raises another interesting point--namely, that use of different fitting routines give different rate constants. However, for k_1 the constants agree with each other within 1 σ if σ is defined by DISCRETE and within 3 σ if σ is defined by the other techniques. Thus, k_1 is probably not significantly different, but for k_2 the difference is larger than 3 σ and the differences appear real.

The DISCRETE fitting routine that we used does not define k_2 with accuracy. The σ values for k_2 as shown in Table 2 vary between 5% and 30% of k_2. This is in contrast to k_1 and A_o which have σ values mostly less than 5% for k_1 and most less than 1% for A_o. The source of the error in k_2 is not clear, but mostly likely has to do with the relative magnitude of k_1 and k_2. For the rate constants presented in Table 2, k_2 exceeds k_1 by an average factor of 4. Thus, chlorohydrin (III) never reaches a significant concentration with respect to mustard (I); that

is, the rate of appearance of chlorohydrin would equal the rate of disappearance when the concentration reaches one-fourth the concentration of mustard. The hydrolysis of chlorohydrin has a small contribution to the overall rate of production of acid. In fact, if k_2 exceeded k_1 by a factor of ~ 10, than the rate would approximate first-order as assumed by many previous workers.[6,18-21]

Ward and Seiders[14] reevaluated the rate constants from the raw data,[18-21] avoiding the assumption of a single first-order rate. However, they failed to get a good fit to consecutive first-order reactions; this was interpreted to mean that some experimental problem existed with the data A second interpretation would be that the kinetics are more complex than the simple consecutive first-order model.

The most likely source of an experimental problem in these experiments is the rate of dissolution of mustard. This rate is reported in the literature to be 1.2×10^{-5} g/cm^2 min.[25] This value is a flux that depends on the surface area, so it is difficult to assess what the actual rate would be. However, making a best guess of a surface area of 10^3 cm^2 gives rate constants on the order of 10^{-3}, and therefore dissolution would be competitive with hydrolysis.

In this study we avoided the problem of dissolution rate by working in mixed solvent systems, which helped avoid the problem in two ways. First, the solubility, and presumably the rate of dissolution, is greater in mixed solvents. Second, we predissolve the mustard with a small amount of the cosolvent so that the rate of dissolution is no longer important. However, the rate of dissolution is replaced by the rate of mixing as an important question. We measured the rate of mixing by observing the mixing time of a similar volume of HCl of an appropriate concentration. These data are shown in Table 8 and Figure 5. The electrode has come to equilibria in ~ 20 sec. Thus the solution should mix in the first 1% of the reaction. This is less than our experimental error in measuring the rate.

Reactions (3) through (6) of Figure 1 show that the reaction is more complicated than consecutive first order. These dimerization reactions could significantly effect the kinetics. As discussed in the Introduction, a reduction in volume ratios of HD/H_2O from 1×10^{-3} to 1×10^{-4} resulted in a drop in dimeric product from 3% to 2.2%. Thus these dimerizations could be effecting the kinetics at the relatively high concentrations used in the previous studies. We avoided this problem by operating at initial mustard concentrations of 6.4×10^{-5} M, where dimerization should account for less than 1% of the product.

The use of these conditions to avoid the problems discussed above entails some compromises. First, the use of mixed solvent systems should lead to slightly slower rates and the activation parameters may also be affected. Second, running the reaction at such low concentrations and avoiding the dissolution problem may not lead to a rate constant that is useful in determining decontamination rates or

Table 8

Data for Mixing of HCl

Time (sec)	$[H^+]$ M
0.83599997E+01	0.54075383E-06
0.15370000E+02	0.57147844E-06
0.29370001E+02	0.58210276E-06
0.50369999E+02	0.58613807E-06
0.78379997E+02	0.58884365E-06
0.13756000E+03	0.59020084E-06
0.16256000E+03	0.59020084E-06
0.22575000E+03	0.58884365E-06

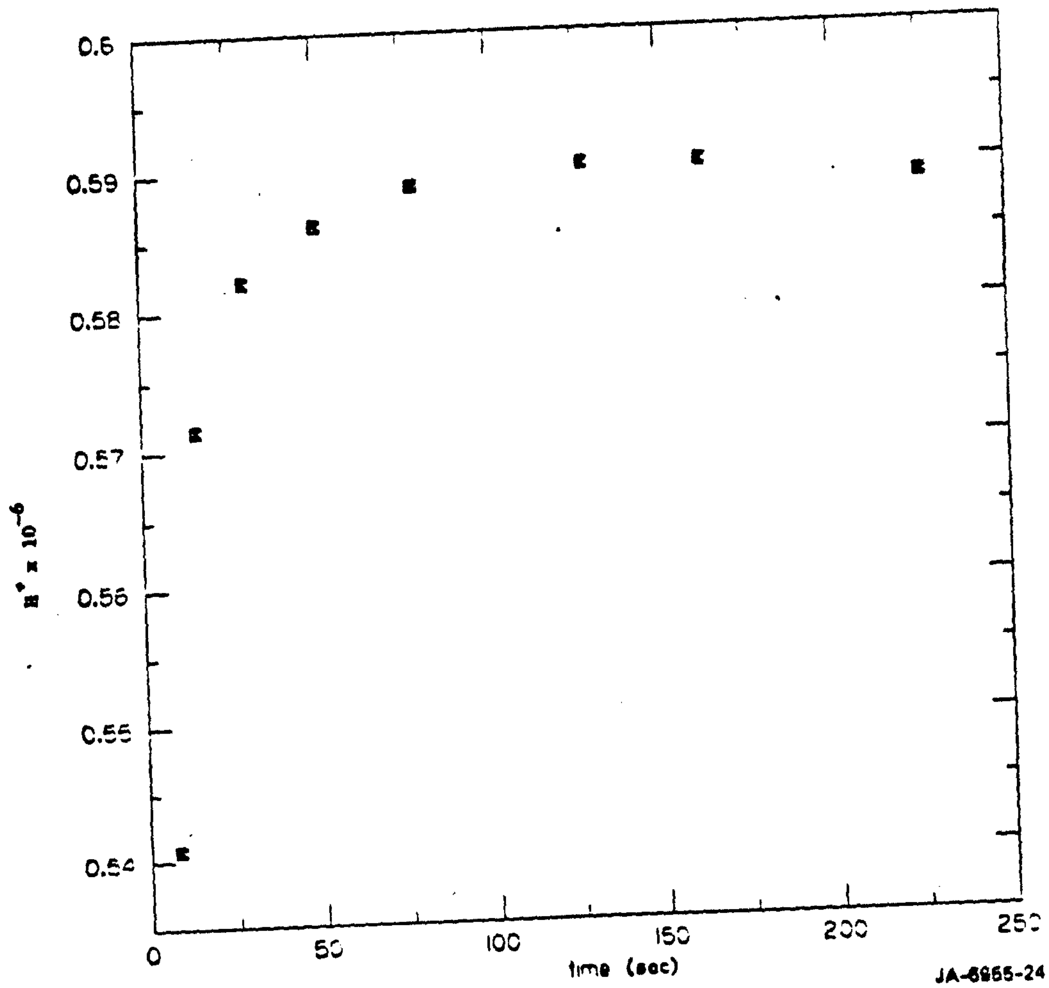

Figure 5. Plot of Data for Mixing of HCl.

environmental lifetimes. The rate constants determined in this way will be accurate for mechanistic considerations, but they must be considered the "best case" (i.e., the fastest rate). However, for environmental fate analysis, rate constants are needed for the "worst case" (i.e., the slowest rate).

The activation parameters can be calculated from the data presented in Table 2 using equation (26) or (27). We found that $\Delta Cp^{\ddagger}$ was not significantly different than zero therefore we used the Arrhenius expression (26) to calculate the activation parameters. These values are presented in Table 9 along with those for several related alkyl halides.[26,27] The arrhenius plots are shown in Figures 6 and 7.

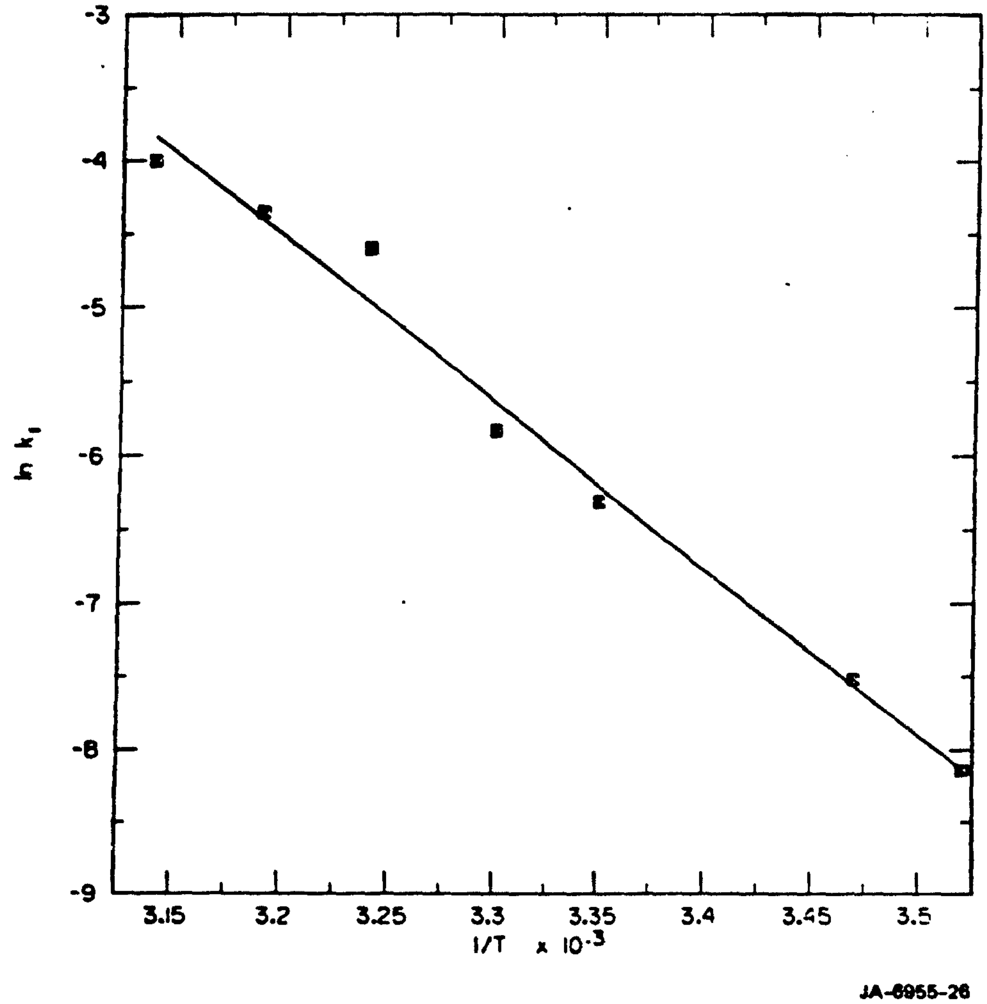

Figure 6. Plot of 1/T vs ln k_1.

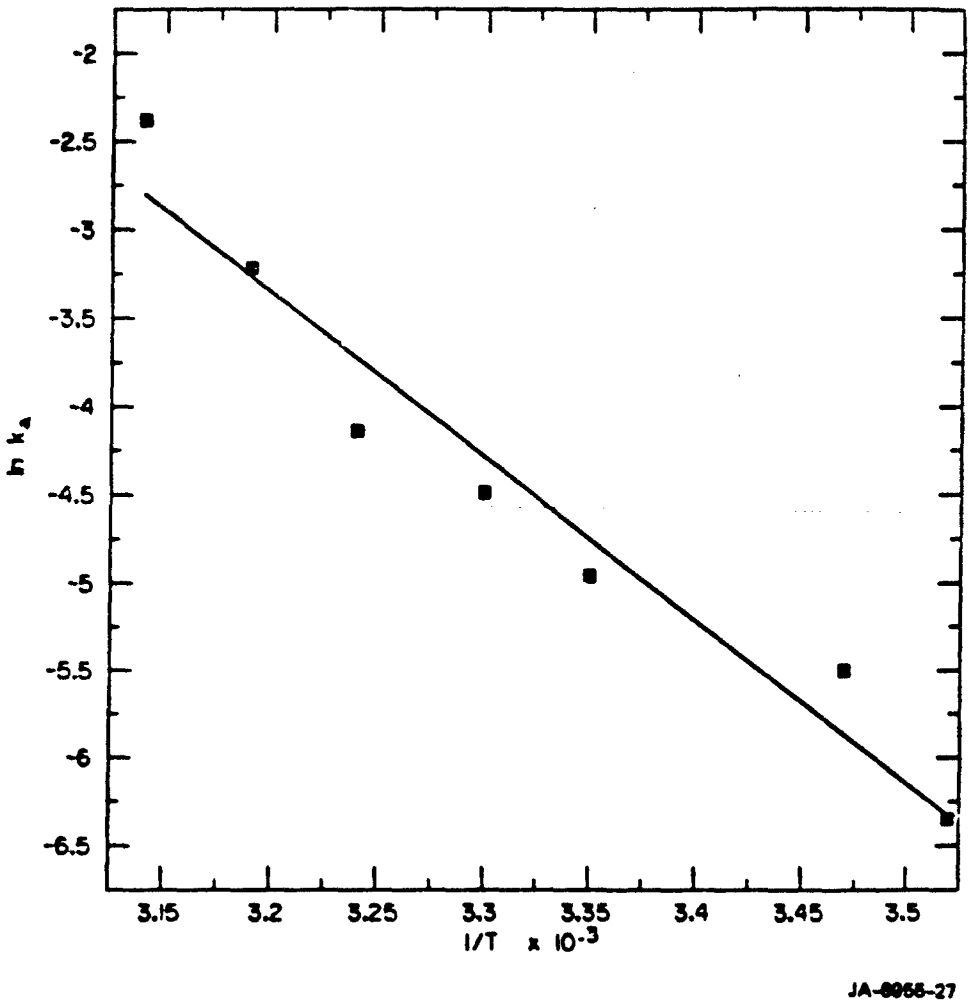

Figure 7. Plot of 1/T vs ln k_2.

Table 9

Comparison of Activation Parameters at 298 K

Compound	Solvent	$k(sec^{-1})$	$\Delta H^{\ddagger}(kcal\ mole^{-1})$	$\Delta C_p^{\ddagger}$(Cal °K mole^{-1}	ΔS(eu)
Mustard[a]	EtOH/water $X = 0.025$	$k_1 = 1.70 \times 10^{-3}$ $k_2 = 6.7 \times 10^{-3}$	25.95 (22.47)[e] 25.23 (18.46)[e]	64.19 61.91	59.68 36.76
Mustard[b]	5% acetone	2.58×10^{-3}			
Cholrohydrin[c]	5% acetone	4.20×10^{-3}	20.7		
CEES[d]	EtOH/water $X = 0.025$	1.61×10^{-2}	20.9	-110	
t-BuCl[d]	EtOH/water $X = 0.025$	2.25×10^{-2}	23.3	-81	

[a]This study.
[b]Bartlett and Swain, Ref. 4.
[c]Harris et al., Ref. 13.
[d]Yang, Ref. 26.
[e]This study calculated from arrhenius plots shown in Figures 6 and 7 with correlation coefficients of 0.99 for k_1 and 0.97 for k_2.

CONCLUSIONS

We have carefully measured the rate of hydrolysis of mustard in mixed EtOH/water over a range of mole fractions from $X = 0.025$ to $X = 0.075$ and a temperature range of 11°C to 45°C. The automated pH stat fabricated to collect this data has proven to be a reliable technique that gives large numbers of data points. The data have been analyzed using a computer technique that fits the data to an exponential series. The best fit of the data is to a two-component exponential series that fits the expected form for consecutive irreversible first-order reactions. The rate constants at 25°C and $X = 0.025$ are $k_1 = 1.70 \times 10^{-3}\ sec^{-1}$ and $k_2 = 6.7 \times 10^{-3}\ sec^{-1}$. Activation parameters are calculated from the data at $X = 0.025$ for each of the two reactions For k_1 $E_a = 22.59$ kcal $mole^{-1}$, ln A = 31.91 and for k_2 $E_a = 25.49$.

These results indicate that the data could be fit to a single first-order rate constant, as assumed by several previous workers, during the early stages of the reaction. However, other problems with earlier data sets, such as dissolution and dimerization problems, are significant, although they did not affect the data collected in this study because the kinetics were measured in mixed solvents at very low concentrations. Thus these data allow the calculation of the most accurate activation parameters for the hydrolysis of mustard reported to date.

Recommendations.

This investigation of the hydrolysis of mustard, due to limitations of time and funding, should not be considered comprehensive. We recommend the following studies to complete a thorough scientific understanding of the hydrolysis of mustard.

More data points should be collected. As pointed out by Moore and Pearson,[22] kinetic runs should be done at least in triplicate rather than the duplicate of the current investigation. The effect of mixed solvents needs to be better defined by measuring in at least two different cosolvents over a wide range of solvent compositions.

Because of the practical considerations discussed earlier, measurements should be made over several orders of magnitude in initial mustard concentration and in compositions with low water content.

Finally, the systematic deviation in the calculated initial mustard concentration should be investigated.

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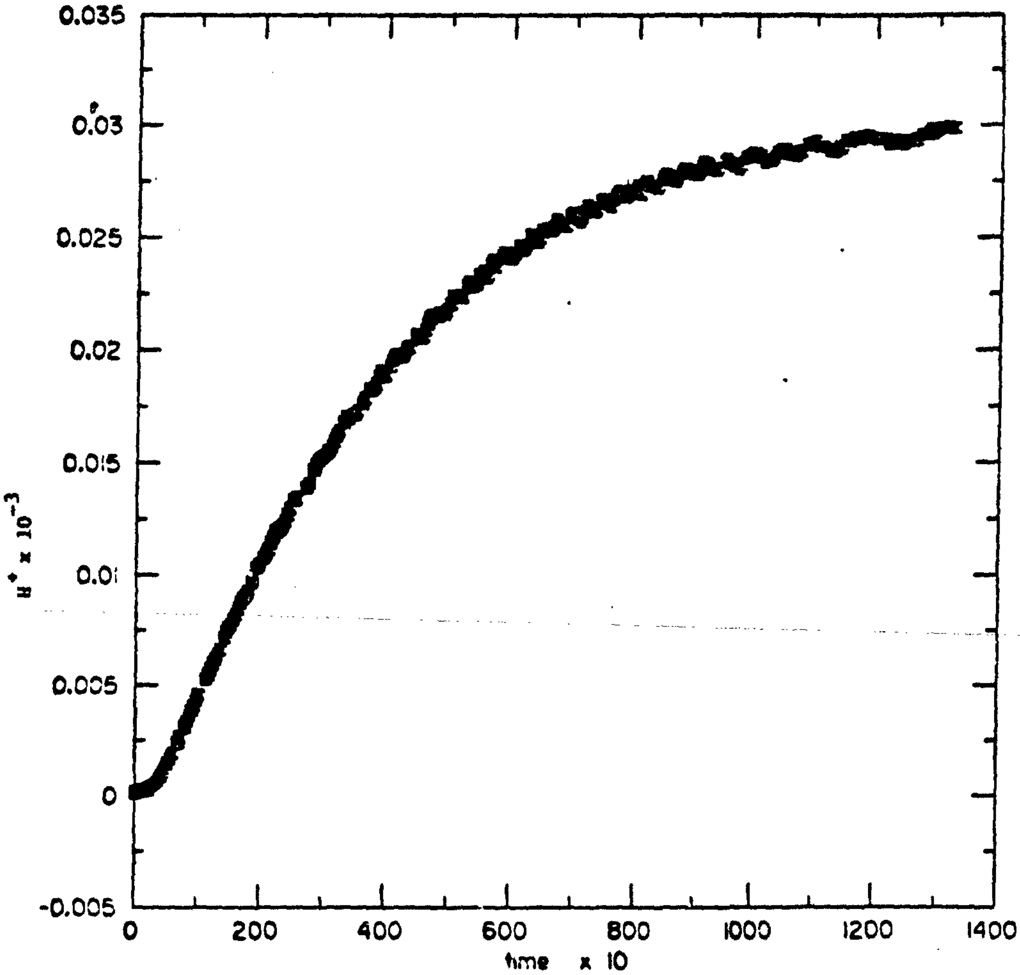
Appendix A

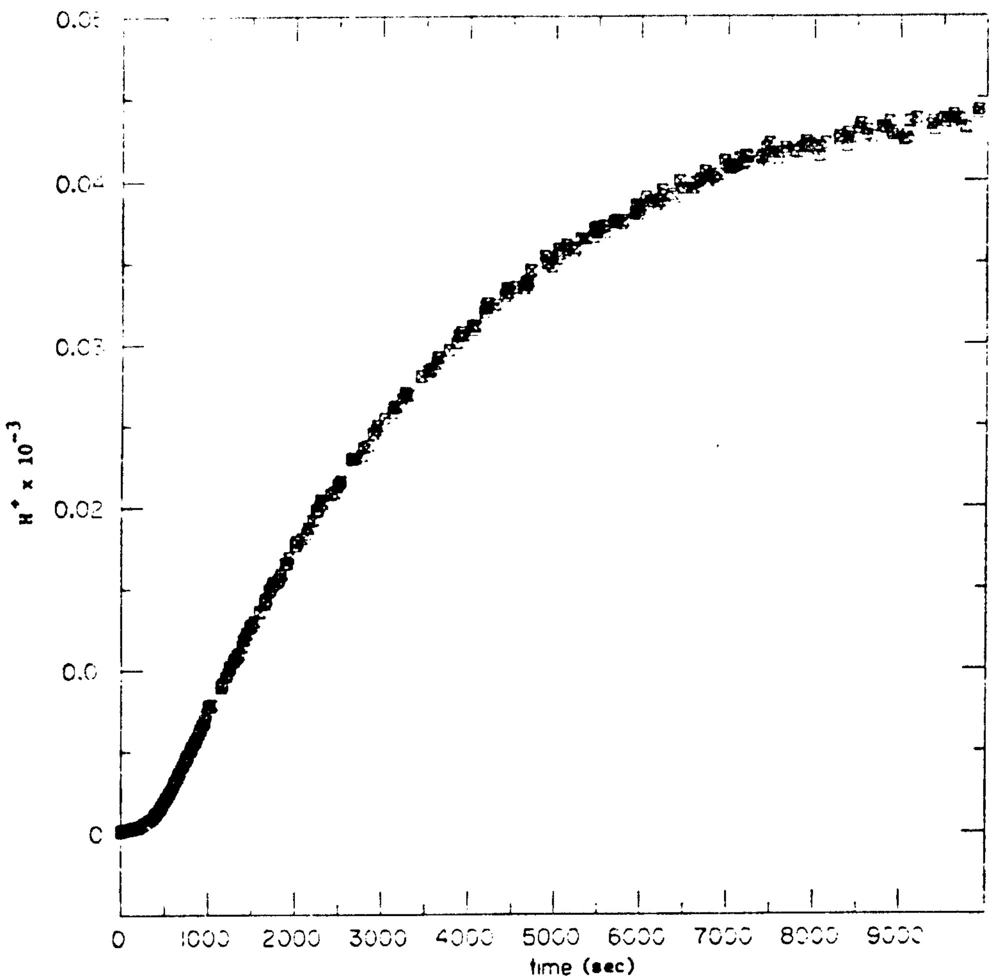
PLOTS OF HYDROLYSIS DATA FOR MUSTARD



(a) Cell One

JA-6955-4

Figure A-1. Plot of Hydrolysis Data for Mustard at 11°C. (Continued)



(b) Cell Two

JA-6955-5

Figure A-1. Plot of Hydrolysis Data for Mustard at 11°C. (Concluded)

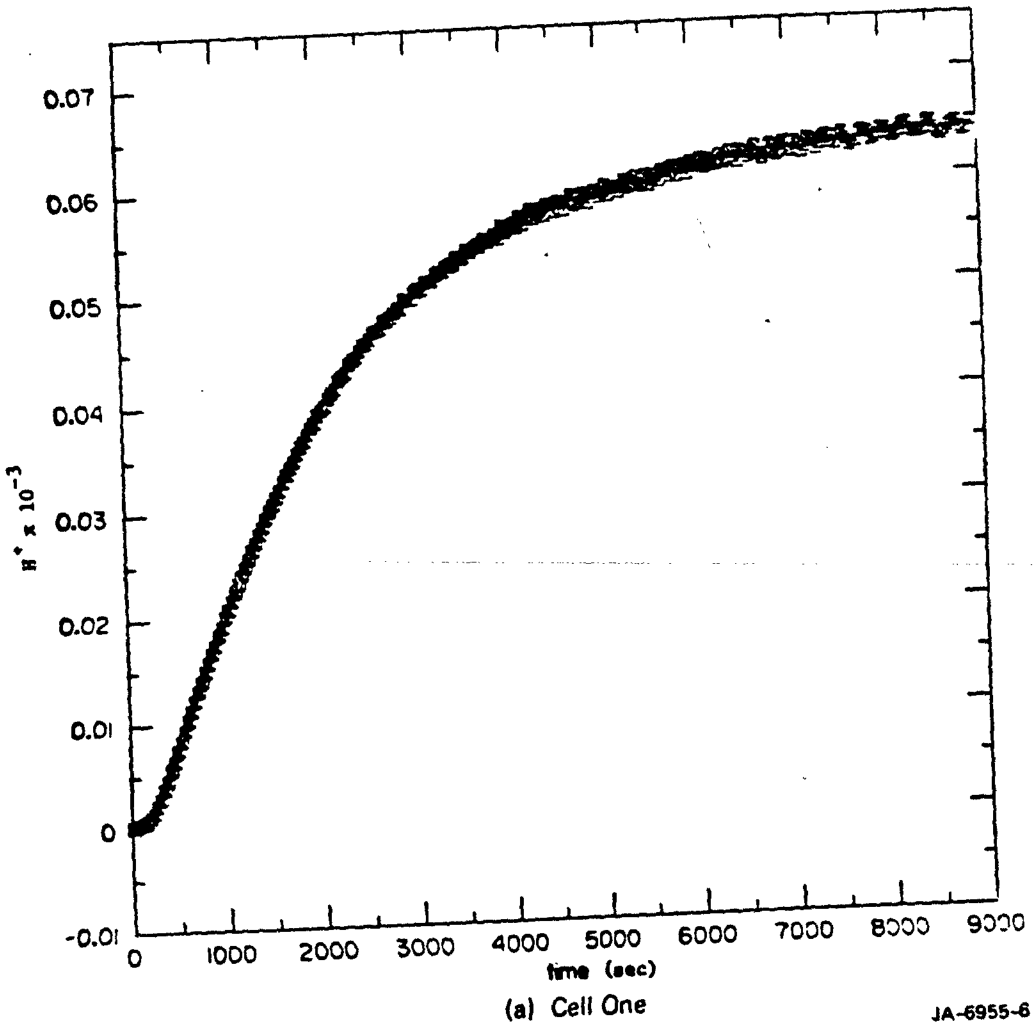
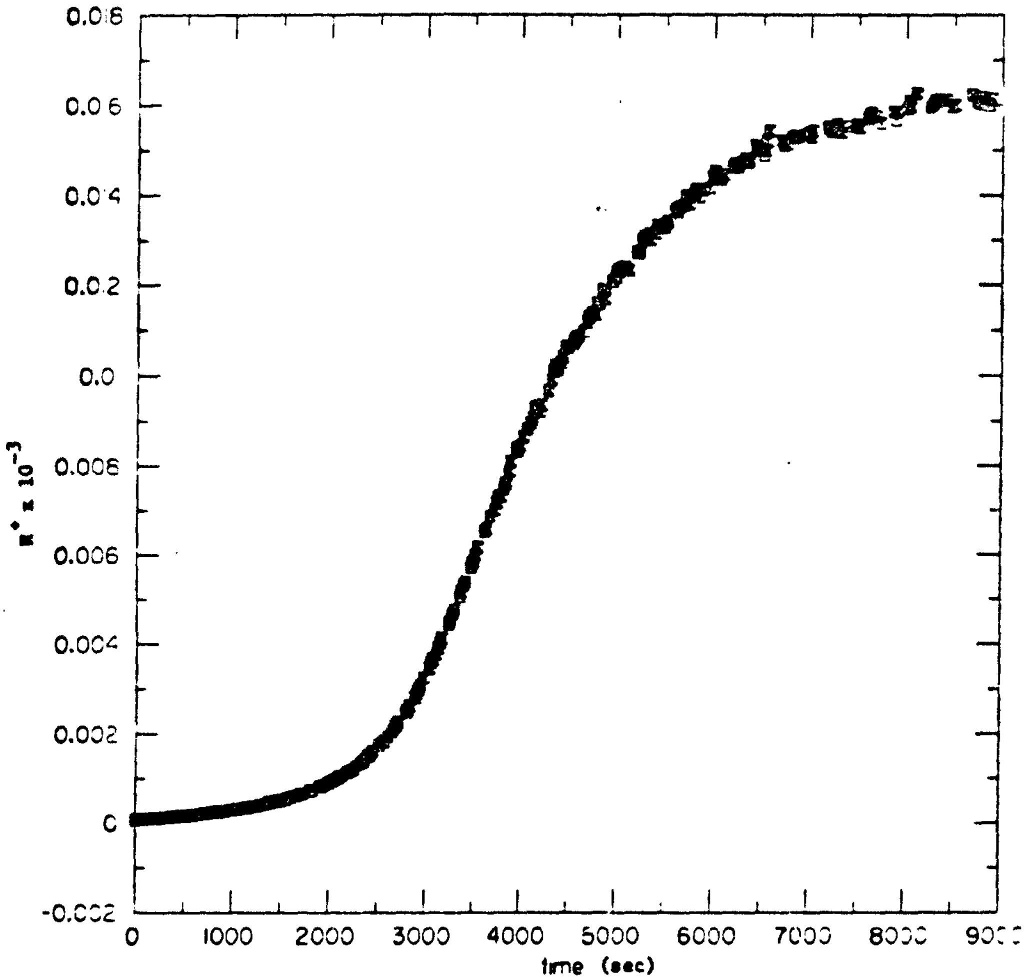


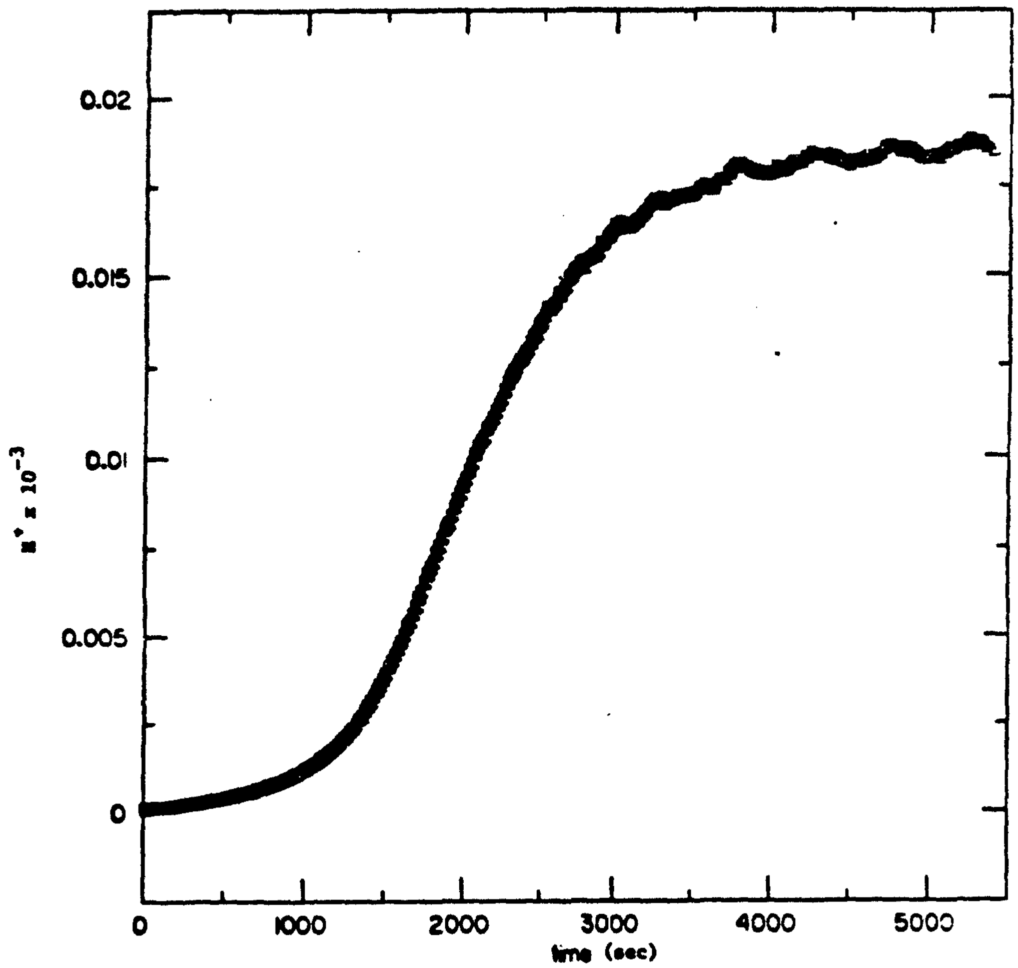
Figure A-2. Plot of Hydrolysis Data for Mustard at 15°C. (Continued)



(b) Cell Two

JA-6955-7

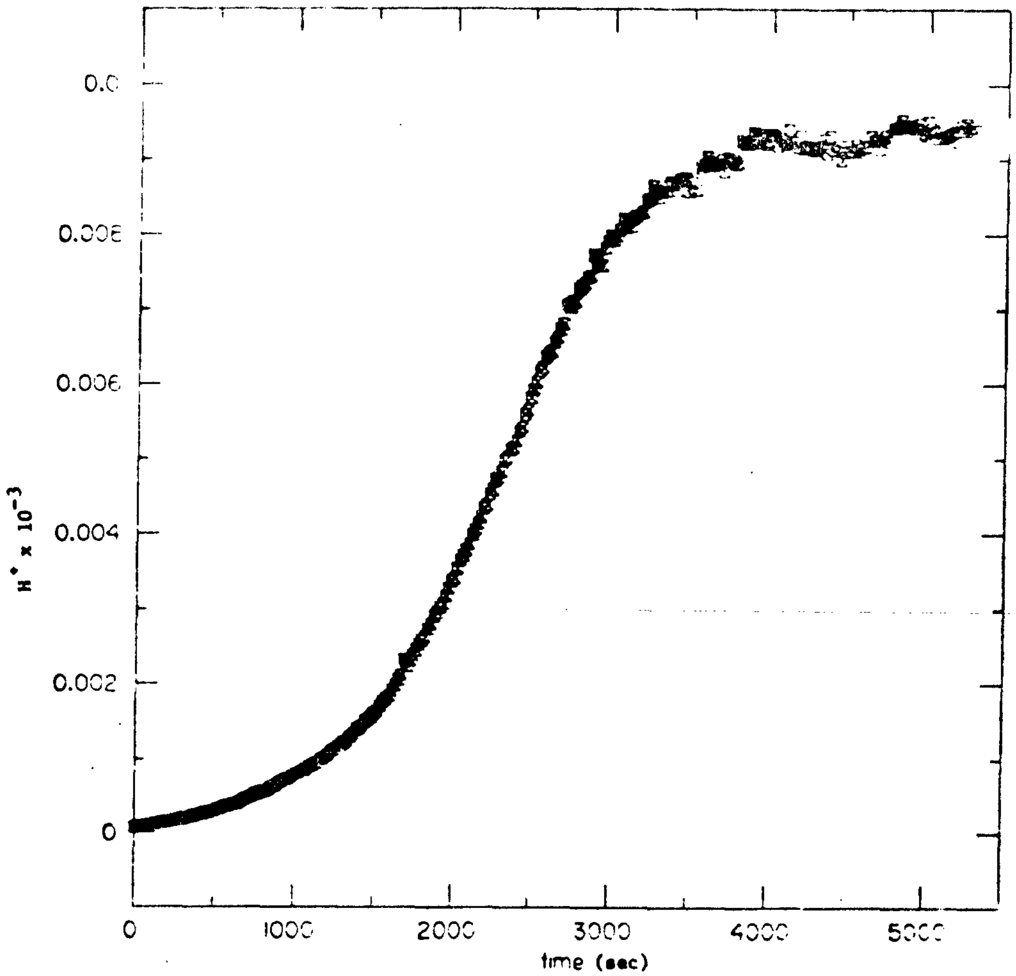
Figure A-2. Plot of Hydrolysis Data for Mustard at 15°C. (Concluded)



(a) Cell One

JA-6955-8

Figure A-3. Plot of Hydrolysis Data for Mustard at 20°C. (Continued)



(b) Cell Two

JA-6955-9

Figure A-3. Plot of Hydrolysis Data for Mustard at 20°C. (Concluded)

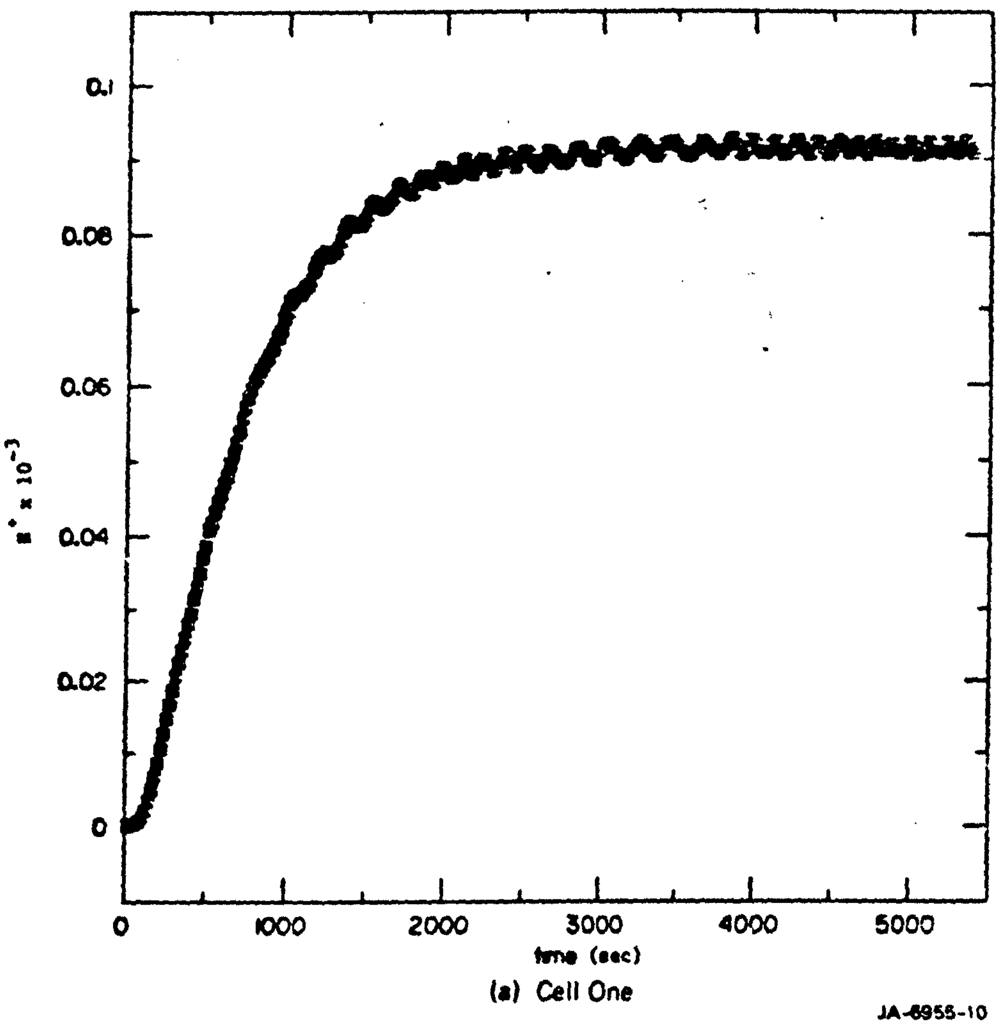
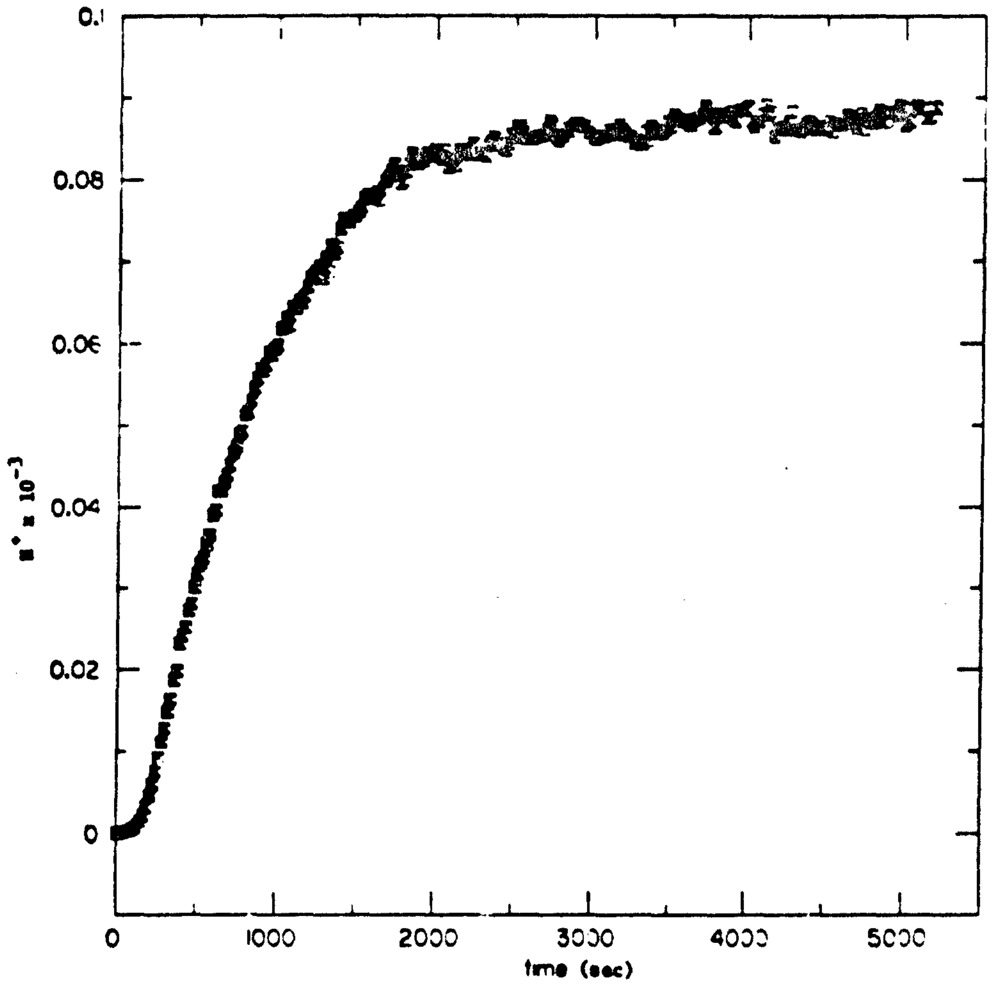


Figure A-4. Plot of Hydrolysis Data for Mustard at 25°C. (Continued)



(b) Cell Two

JA-6955-11

Figure A-4. Plot of Hydrolysis Data for Mustard at 25°C. (Concluded)

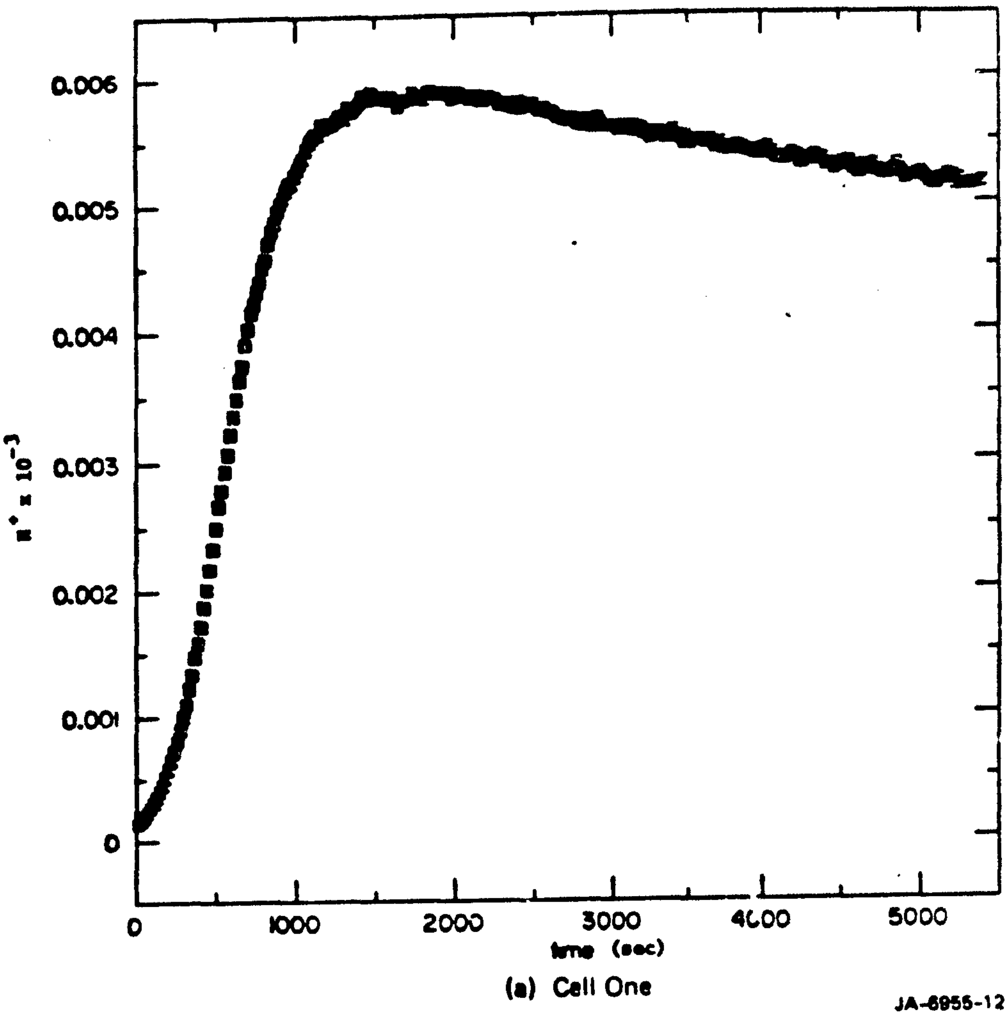
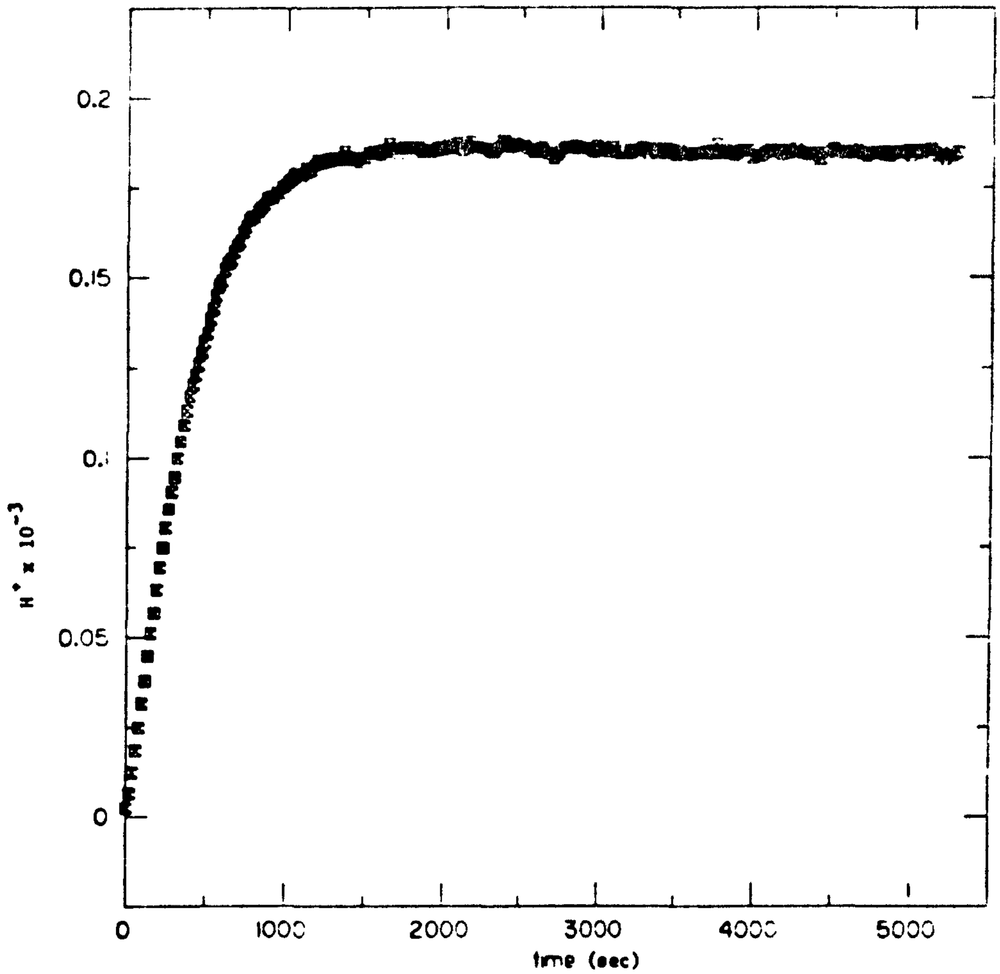


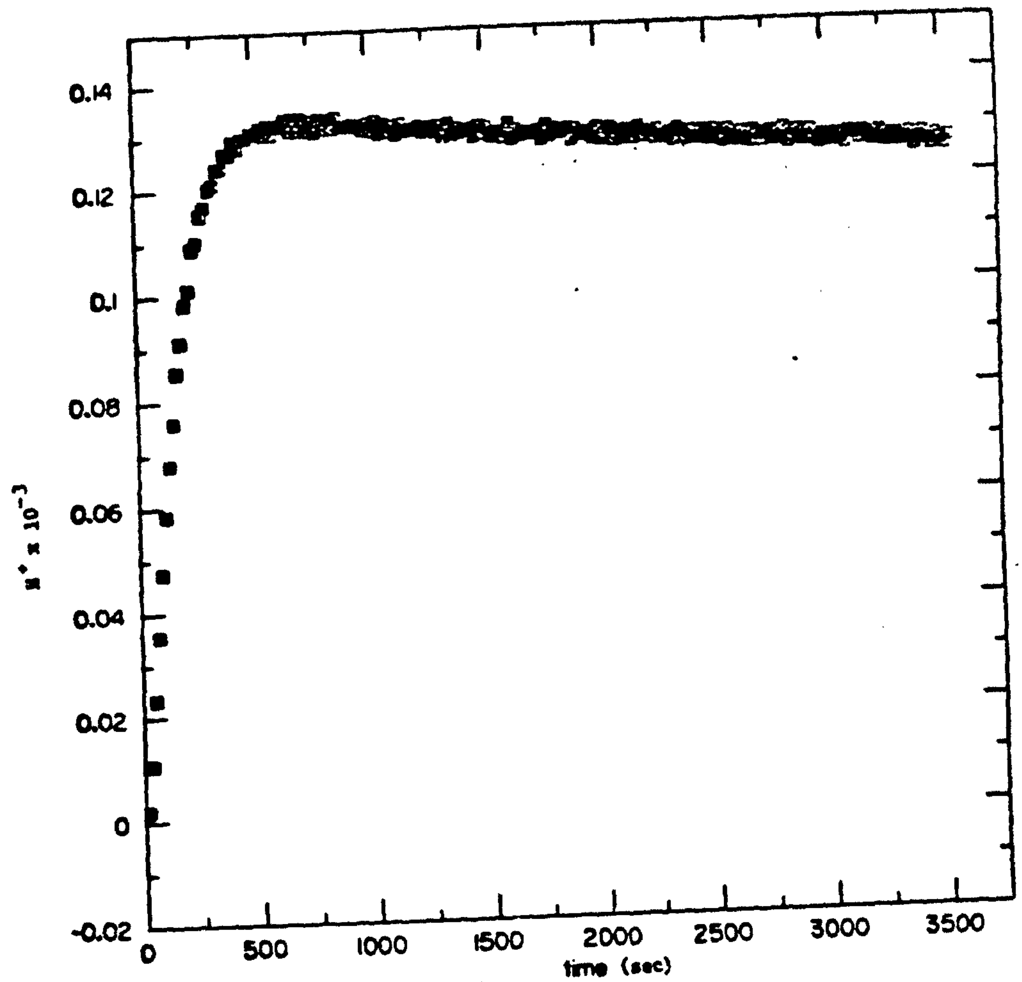
Figure A-5. Plot of Hydrolysis Data for Mustard at 30°C.
(Continued)



(b) Cell Two

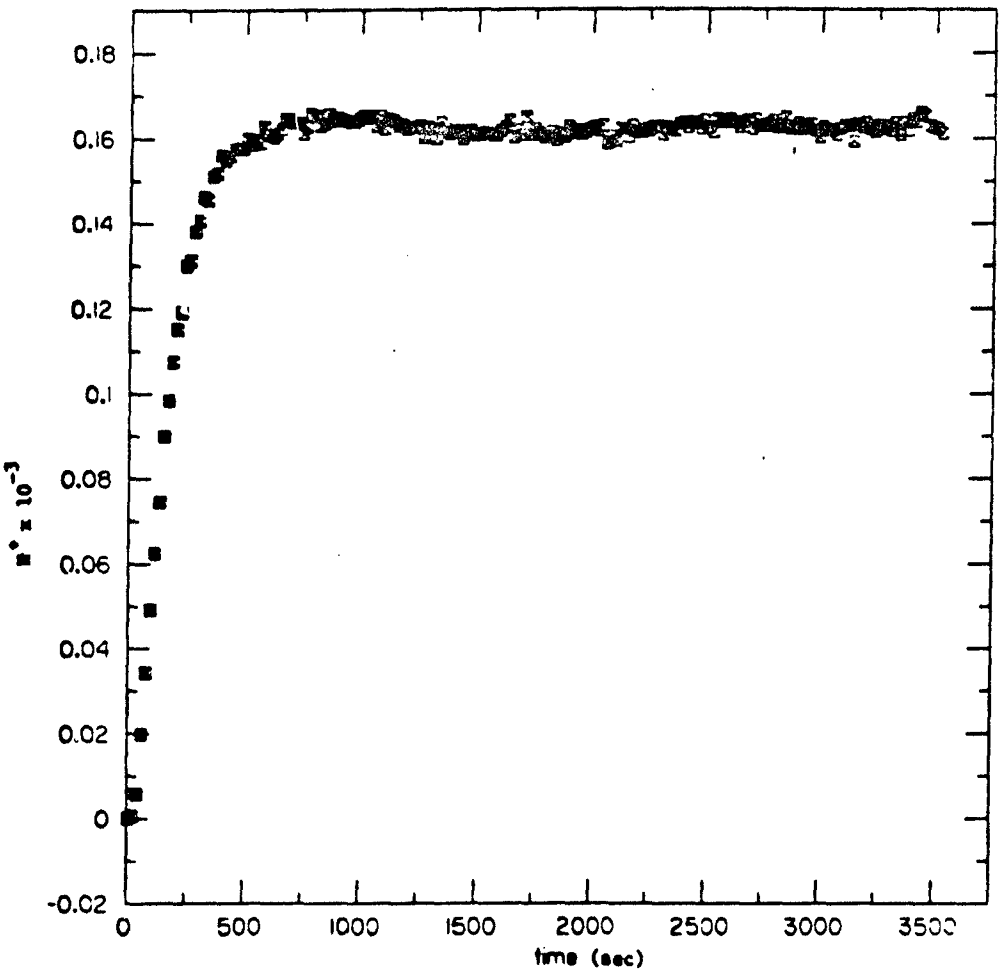
JA-6955-13

Figure A-5. Plot of Hydrolysis Data for Mustard at 30°C. (Concluded)



(a) Cell One

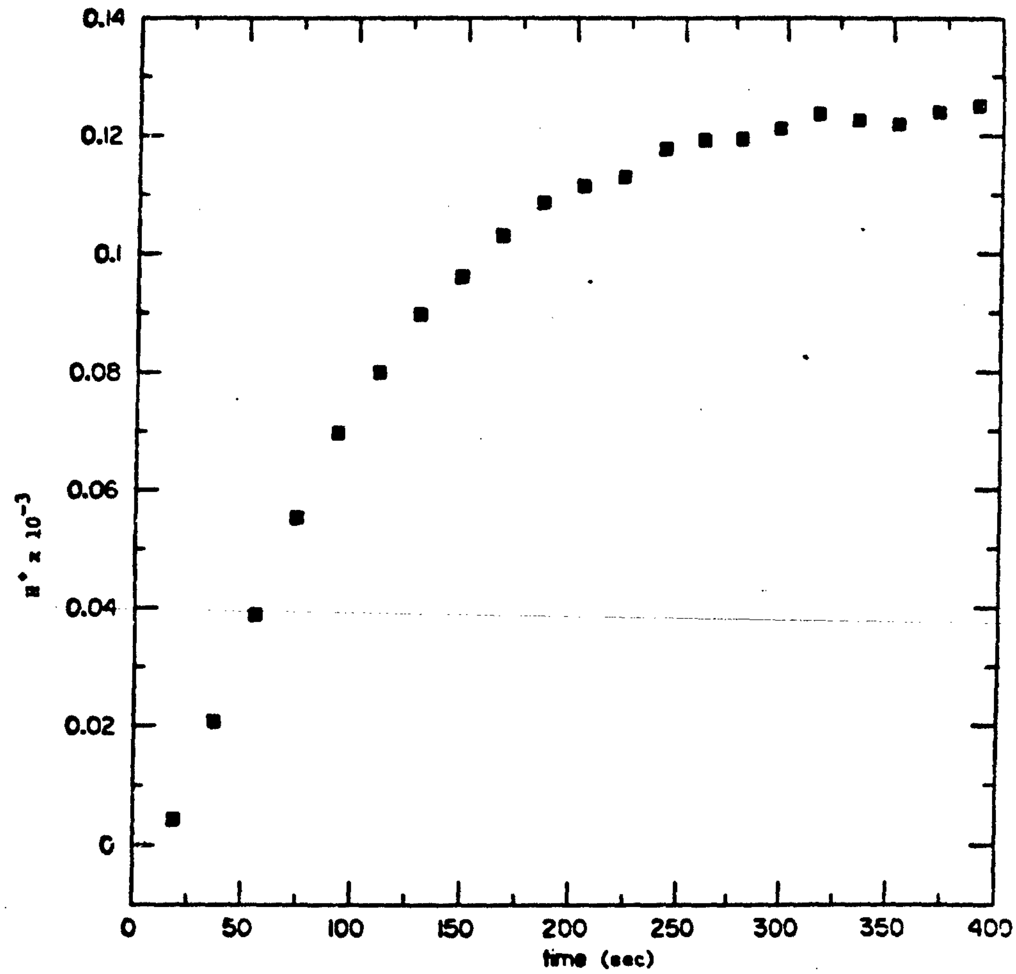
Figure A-6. Plot of Hydrolysis Data for Mustard at 35°C. (Continued)



(b) Cell Two

JA-6955-15

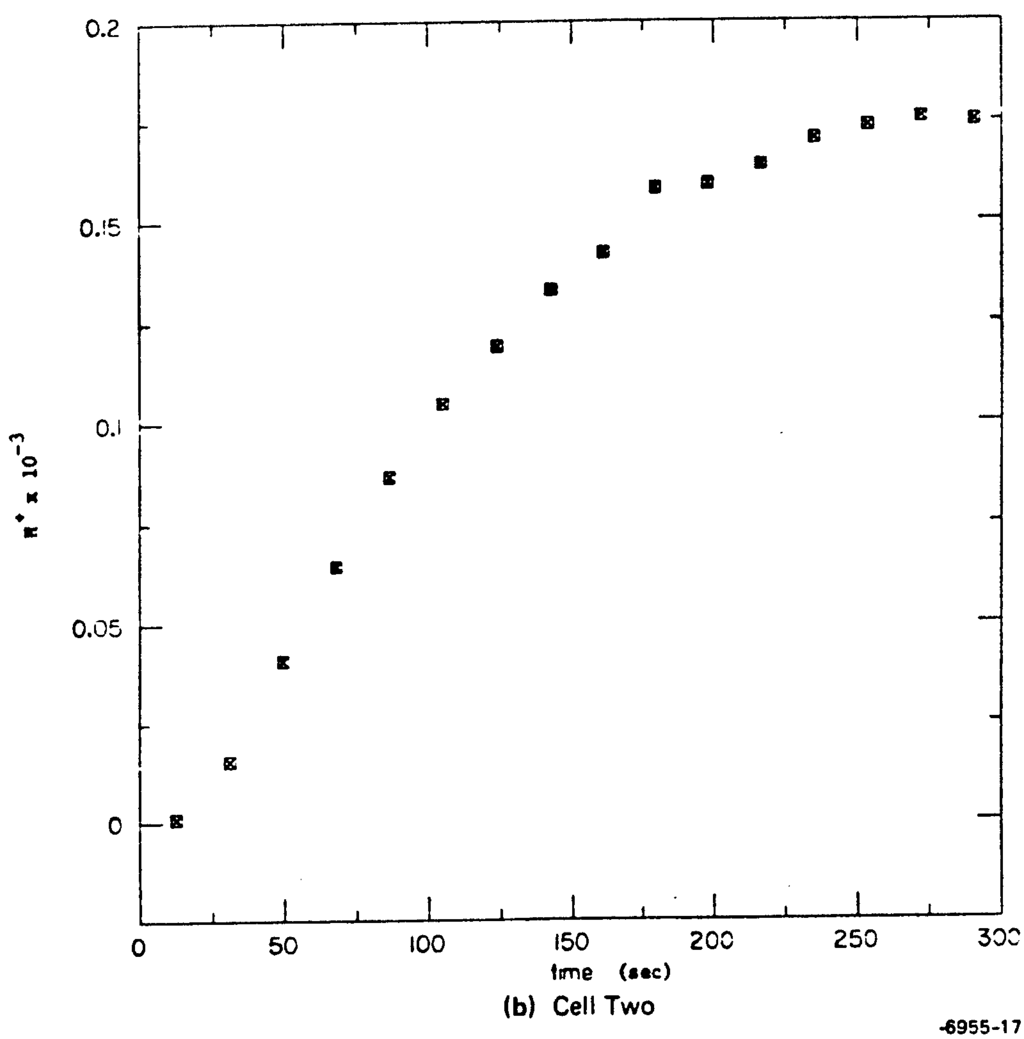
Figure A-6. Plot of Hydrolysis Data for Mustard at 35°C. (Concluded)



(a) Cell One

JA-6955-16

Figure A-7. Plot of Hydrolysis Data for Mustard at 40°C. (Continued)



(b) Cell Two

Figure A-7. Plot of Hydrolysis Data for Mustard at 40°C. (Concluded)

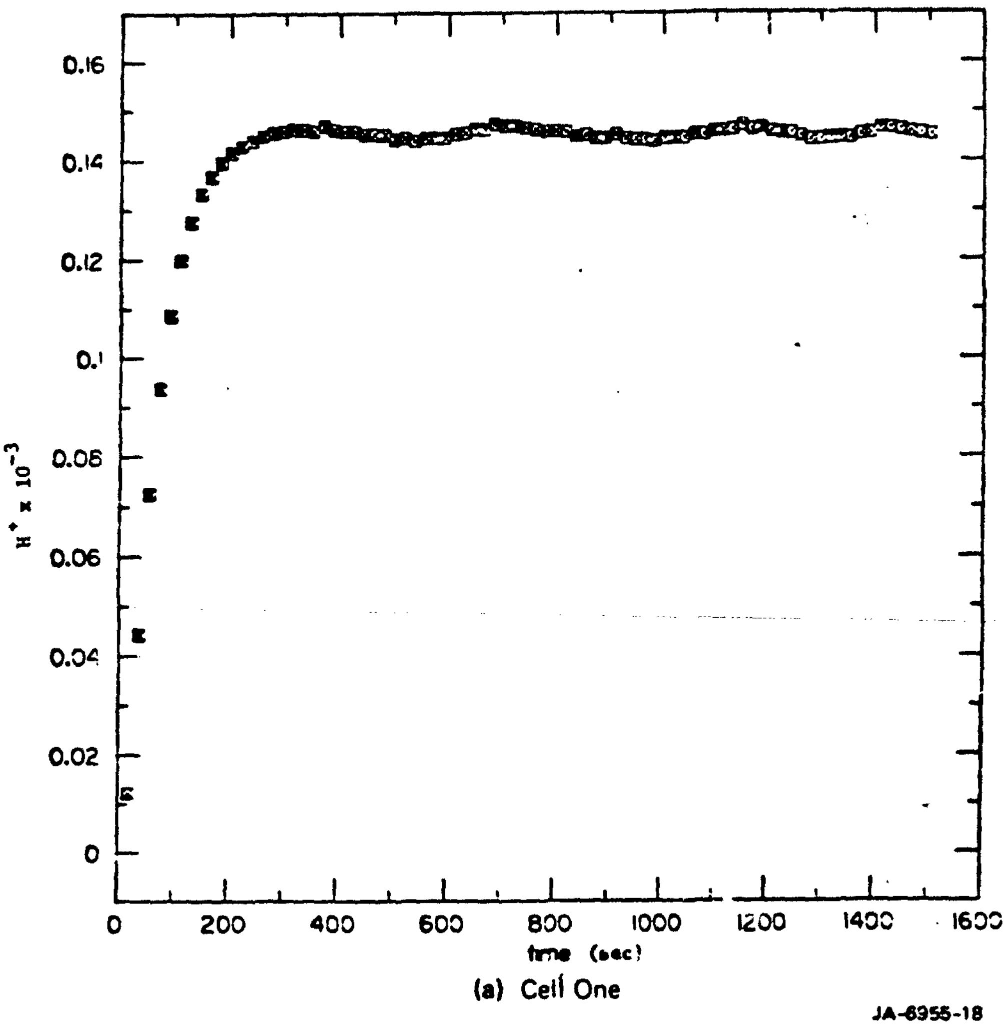
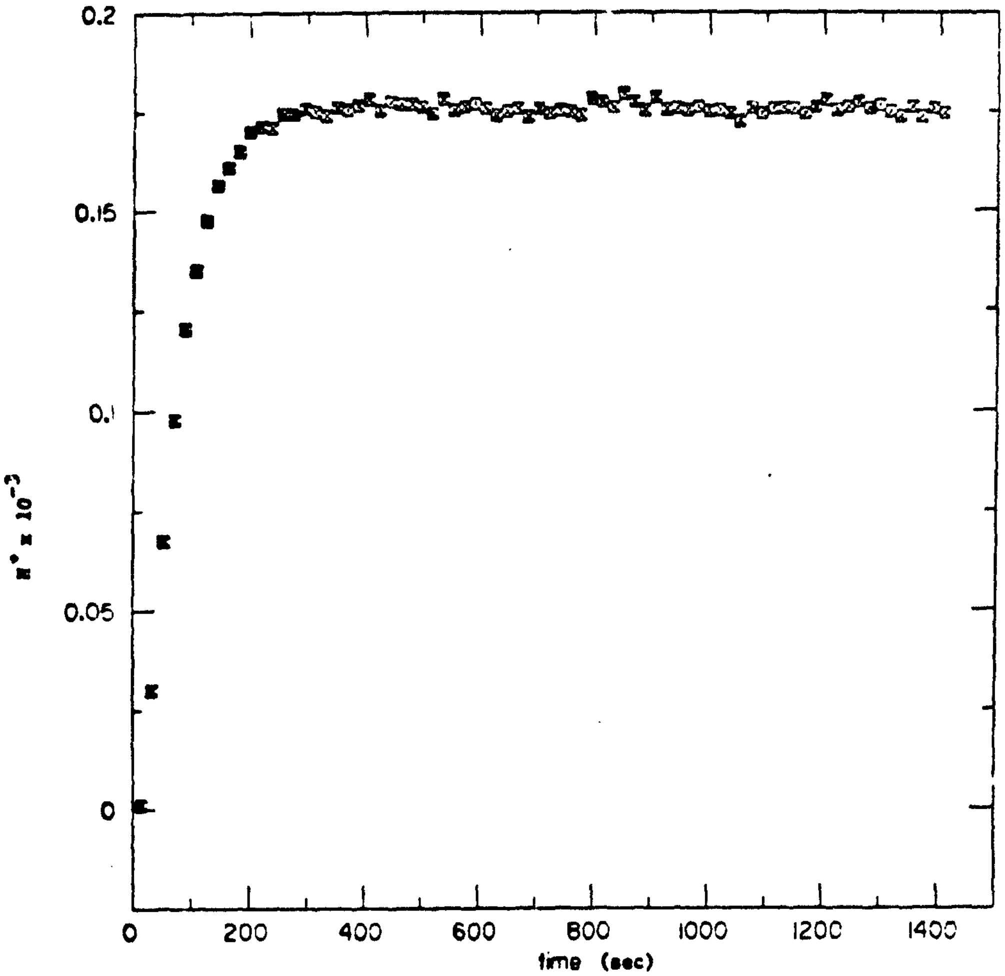


Figure A-8. Plot of Hydrolysis Data for Mustard at 45°C. (Continued)



(b) Cell Two

JA-695_-19

Figure A-8. Plot of Hydrolysis Data for Mustard at 45°C. (Concluded)

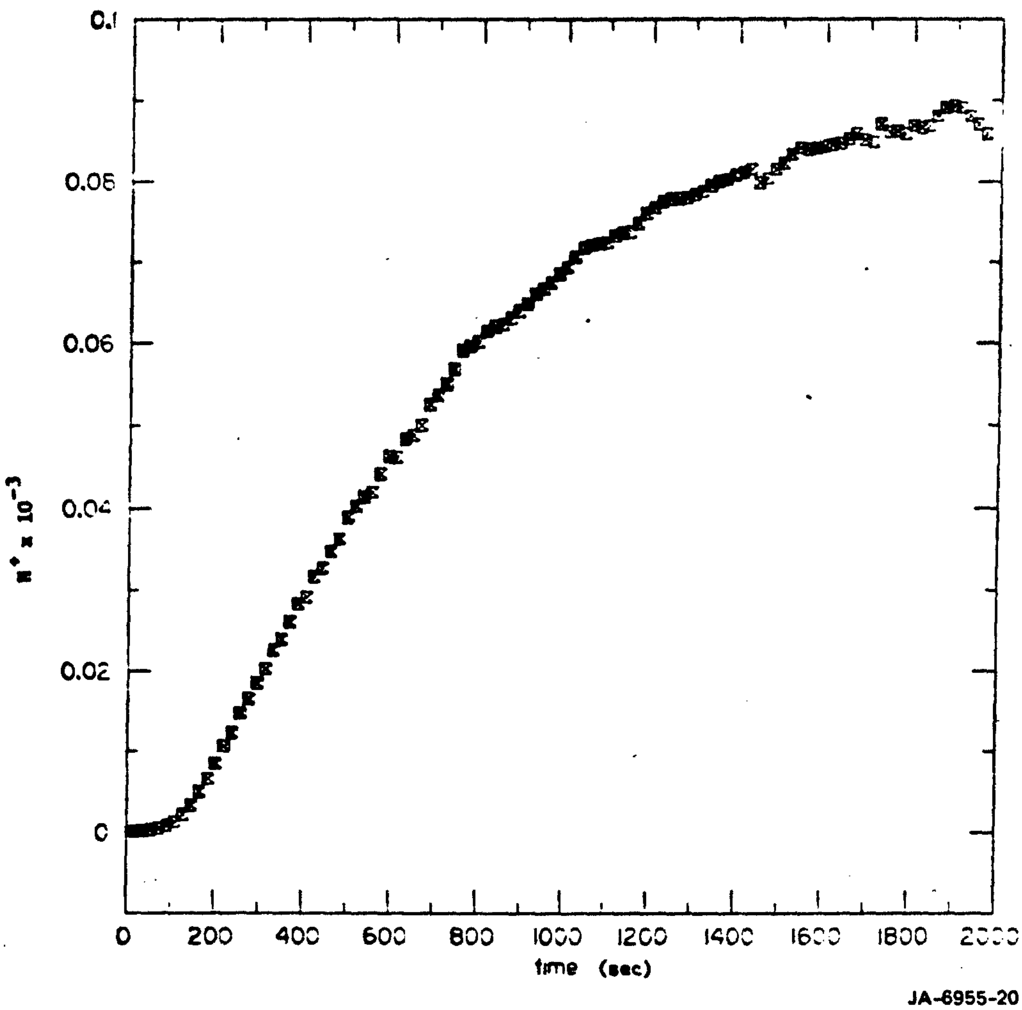


Figure A-9. Plot of Hydrolysis Data for Mustard at 25°C and 0.05 Mole Fraction Ethanol.

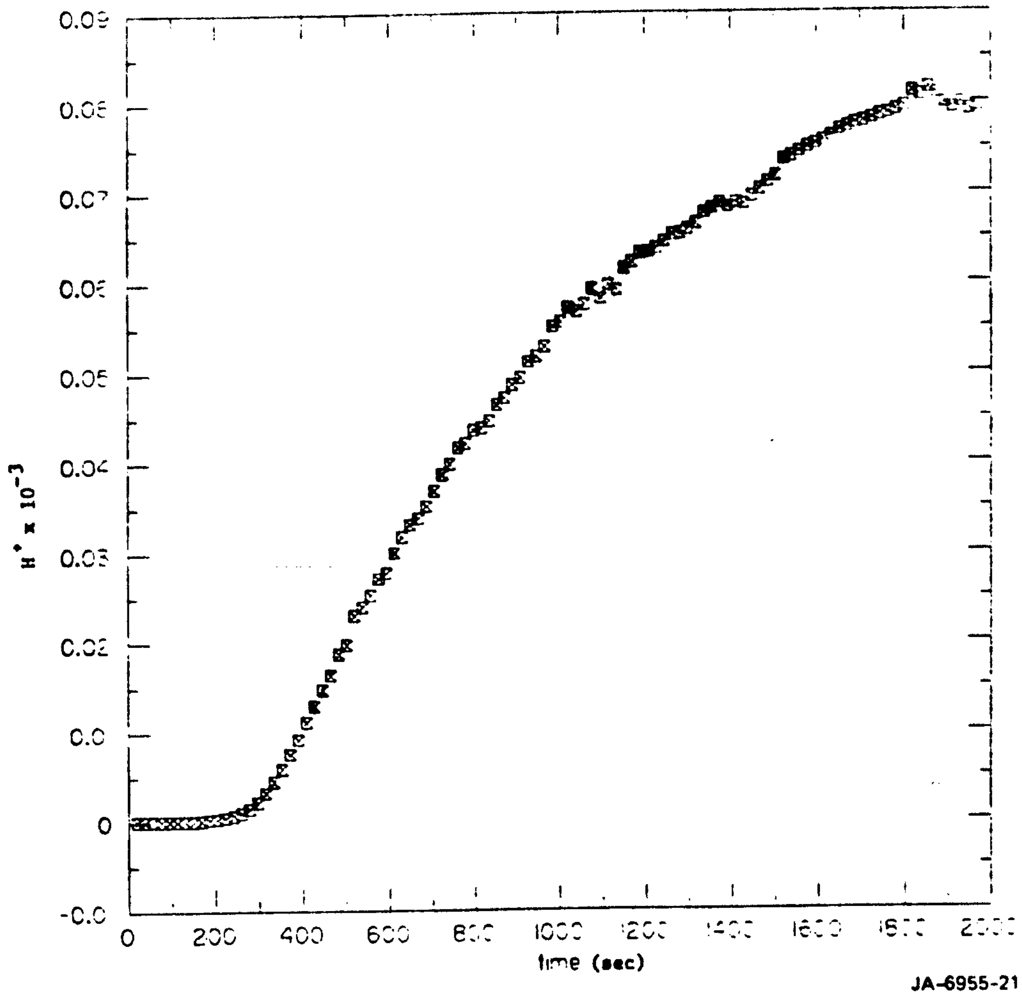


Figure A-10. Plot of Hydrolysis Data for Mustard at 25°C and 0.075 Mole Fraction Ethanol.

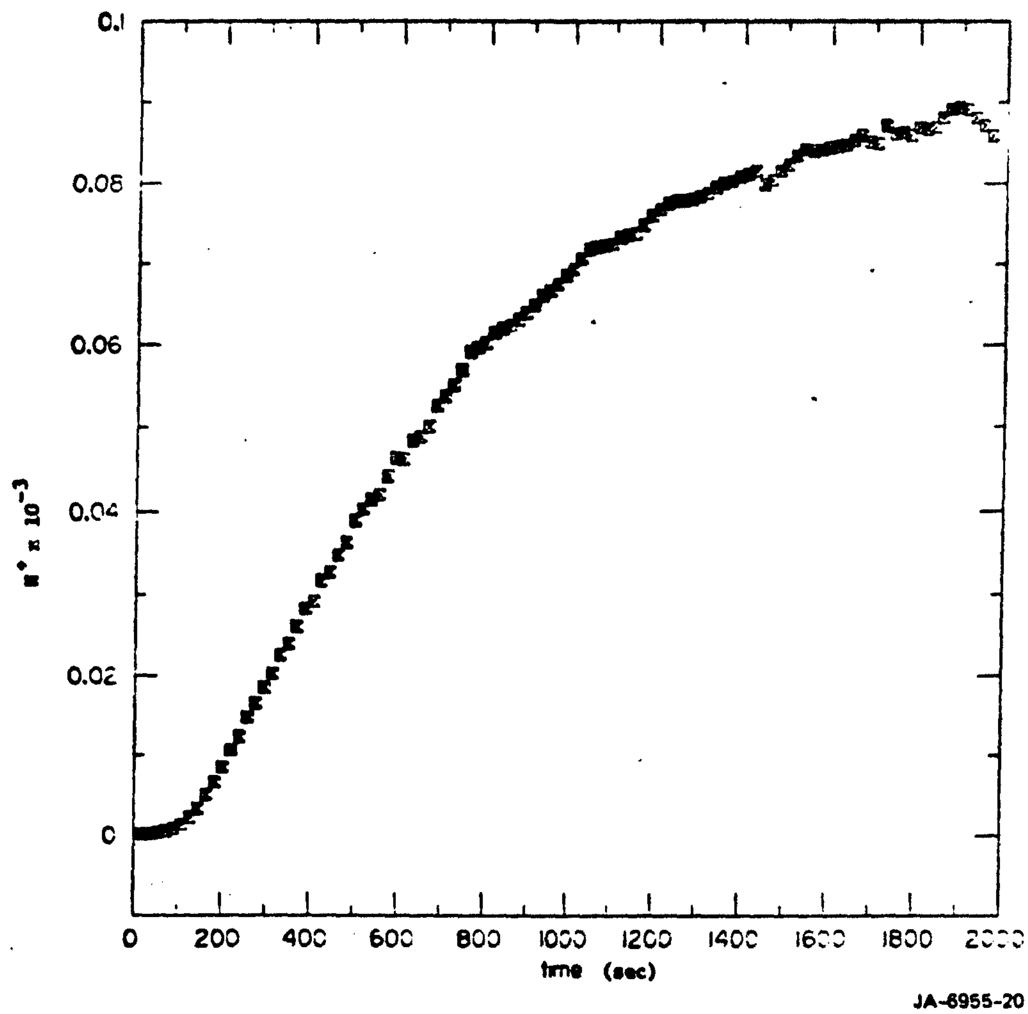


Figure A-9. Plot of Hydrolysis Data for Mustard at 25°C and 0.05 Mole Fraction Ethanol.

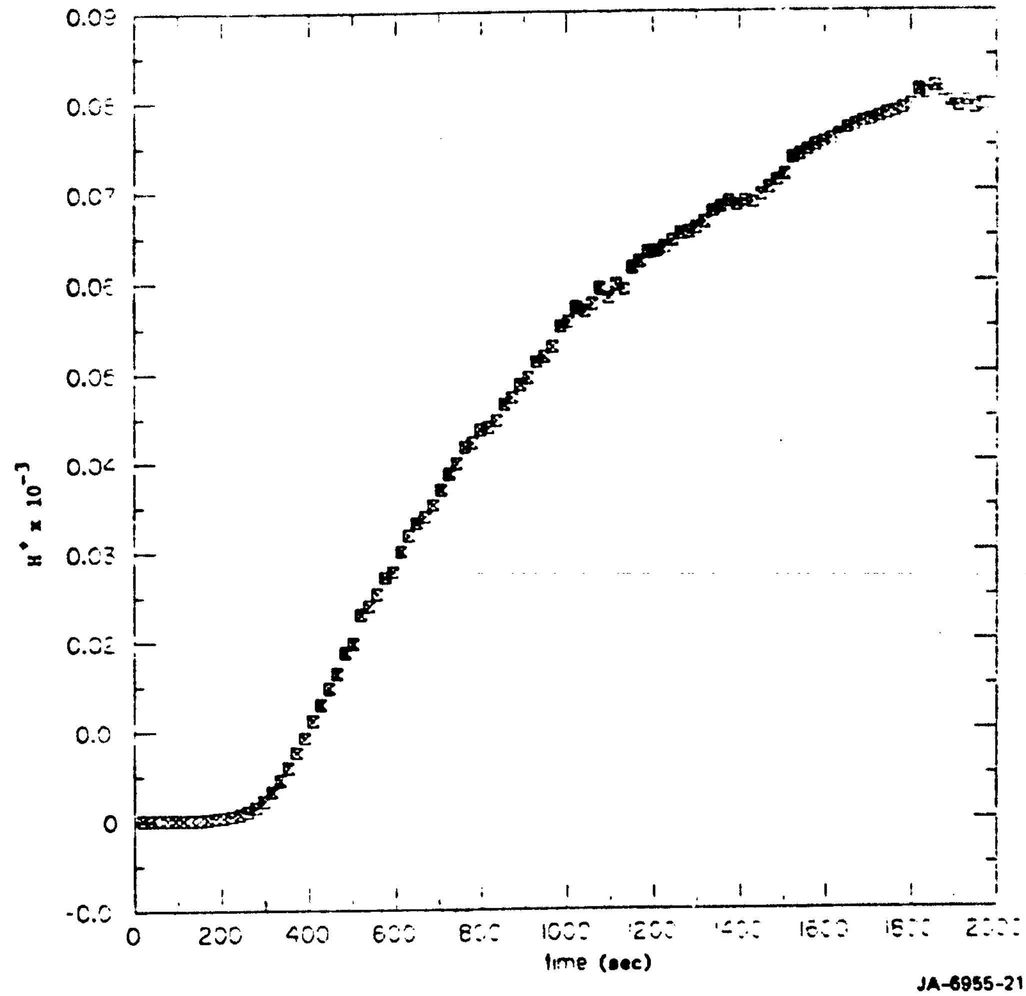


Figure A-10. Plot of Hydrolysis Data for Mustard at 25°C and 0.075 Mole Fraction Ethanol.

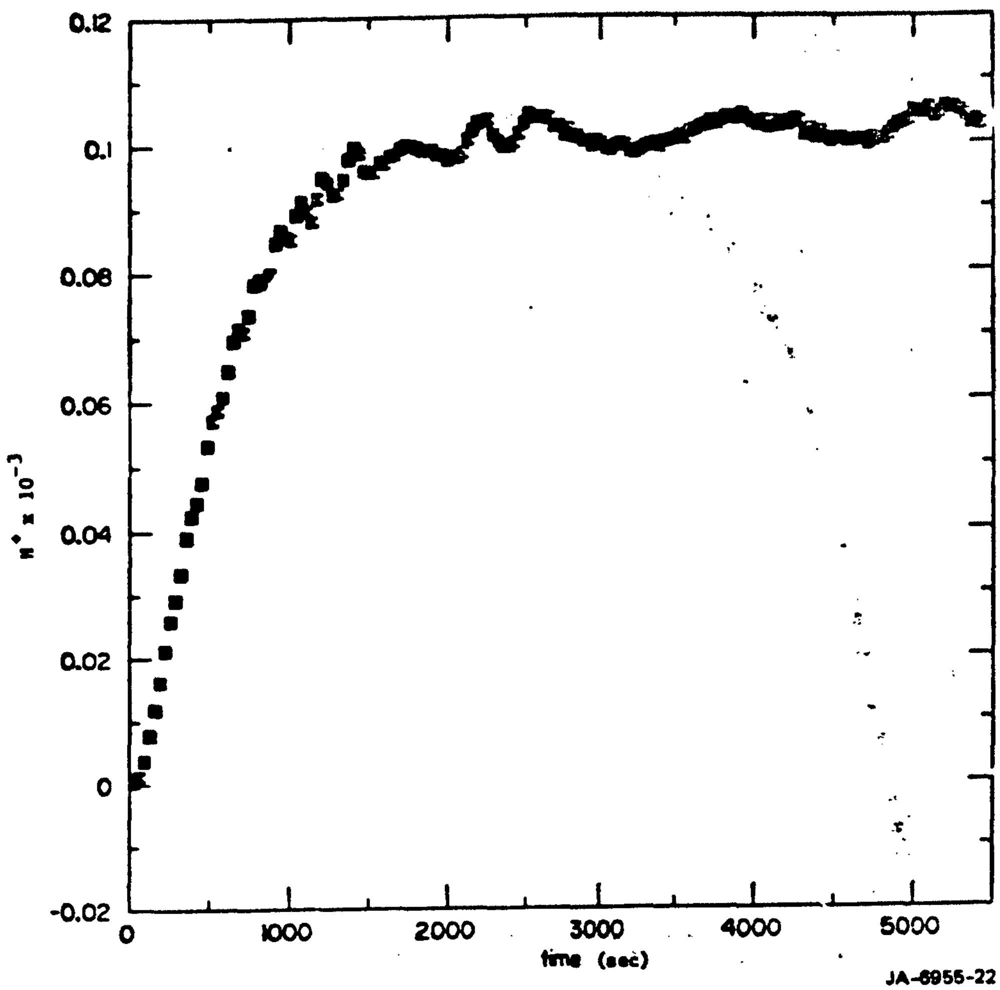


Figure A-11. Plot of the Hydrolysis of Mustard in 5% Acetone at 25°C.

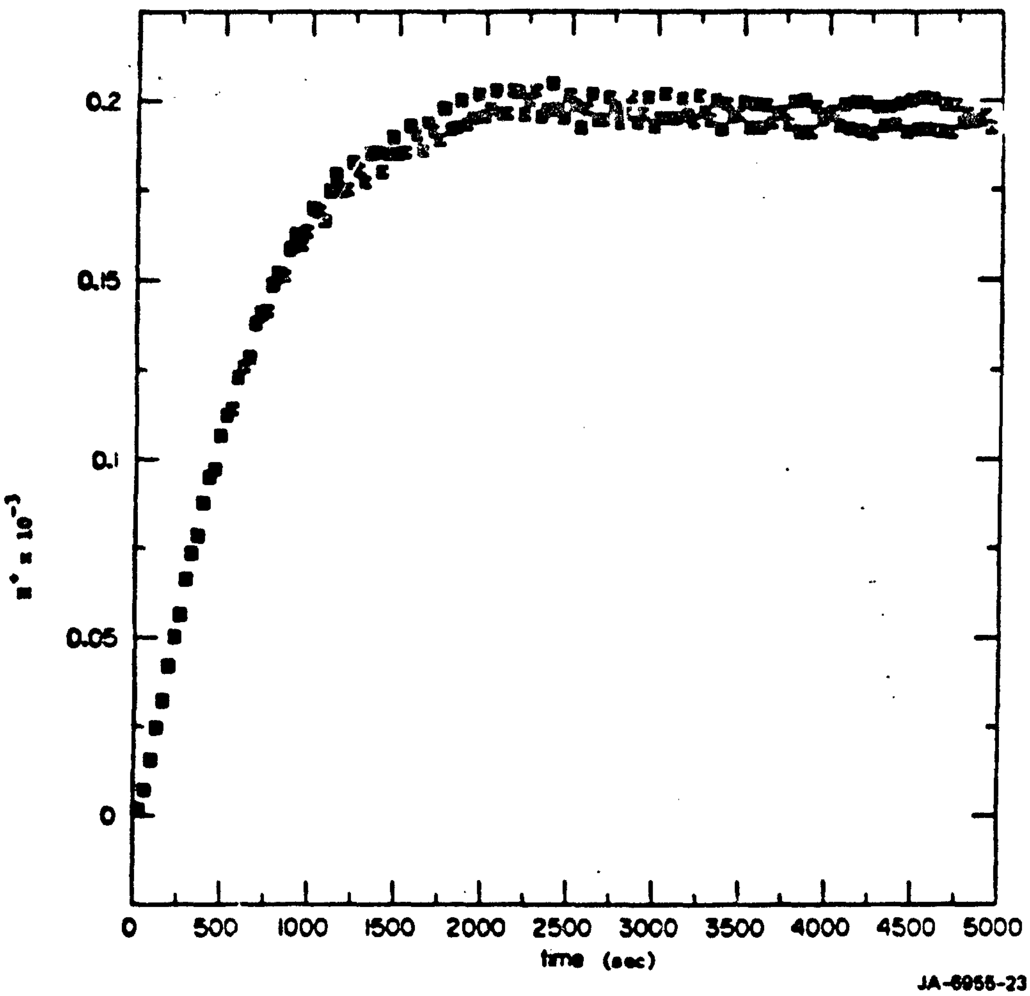


Figure A-12. Plot of Hydrolysis Data for Mustard in 0.025 X EtOH/Water at 25°C and Twice the Initial Mustard Concentration.

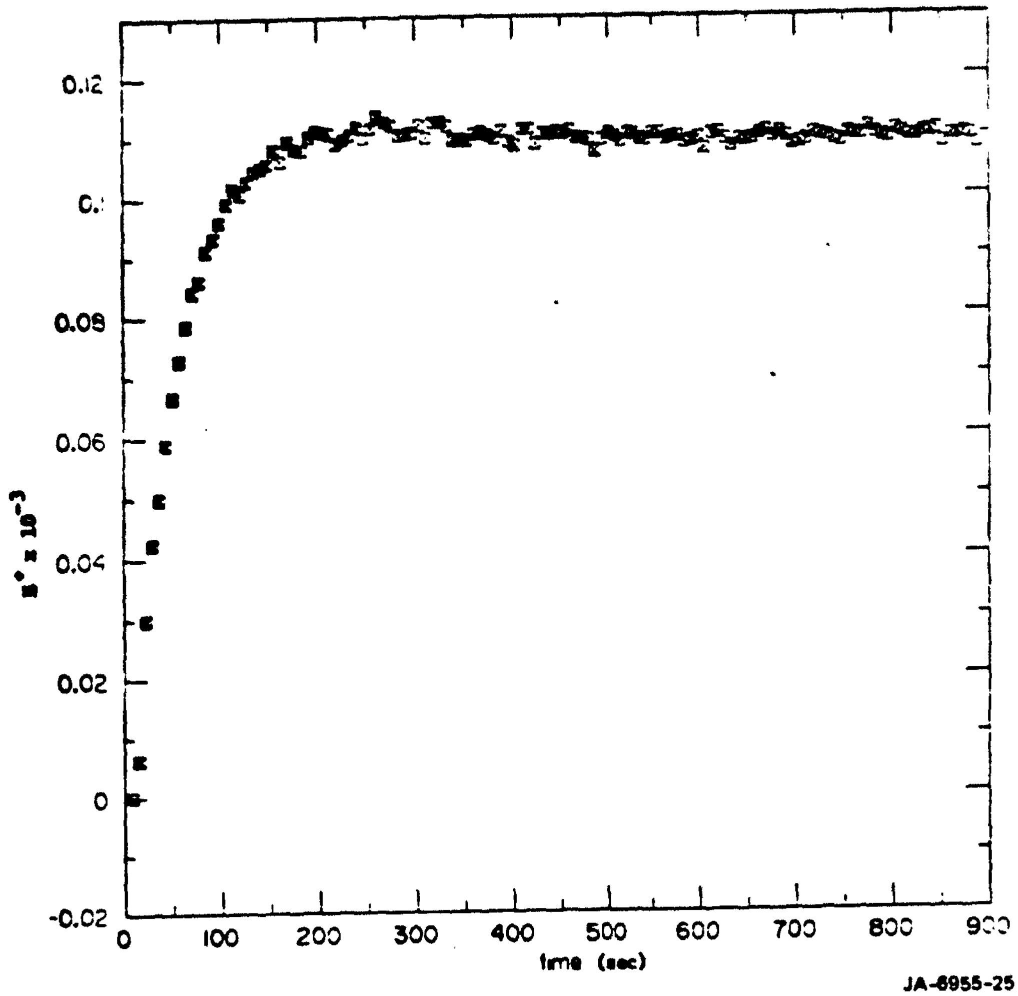


Figure A-13. Plot of Hydrolysis Data for Chloroethyl Ethyl Sulfide in 5% Acetone/Water (V/V) at 25°C.

Appendix B

TABLES OF DATA FOR MUSTARD HYDROLYSIS AT VARIOUS TEMPERATURES

Table B-1

Data for Mustard Hydrolysis at 284 K

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.18700001E+02	0.12793809E-06
0.55700001E+02	0.16788029E-06
0.92690002E+02	0.19014778E-06
0.12969000E+03	0.21677040E-06
0.16667999E+03	0.26121600E-06
0.20367999E+03	0.31045596E-06
0.24117999E+03	0.35481332E-06
0.27817001E+03	0.42657948E-06
0.31517001E+03	0.51760702E-06
0.35216000E+03	0.61517070E-06
0.38916000E+03	0.72276993E-06
0.42614999E+03	0.86096173E-06
0.46314999E+03	0.10423174E-05
0.50082001E+03	0.12331051E-05
0.53781000E+03	0.14354900E-05
0.57479999E+03	0.16034135E-05
0.61179999E+03	0.18923439E-05
0.68578998E+03	0.23713726E-05
0.72345001E+03	0.26242194E-05
0.79744000E+03	0.31045613E-05
0.83442999E+03	0.33496549E-05
0.87142999E+03	0.35892162E-05
0.90841998E+03	0.38222474E-05
0.94541998E+03	0.40350817E-05
0.98308002E+03	0.43052651E-05
0.10201000E+04	0.45289762E-05
0.11311000E+04	0.52723009E-05
0.11681000E+04	0.54827642E-05
0.12051000E+04	0.57147872E-05
0.12427000E+04	0.59703520E-05
0.12797000E+04	0.61801602E-05
0.13167000E+04	0.63826301E-05
0.13537000E+04	0.66069392E-05
0.14277000E+04	0.71449626E-05
0.14652000E+04	0.74473205E-05
0.15022000E+04	0.76383531E-05
0.15392000E+04	0.77624654E-05
0.15762000E+04	0.79799474E-05
0.16132000E+04	0.82035140E-05
0.16502000E+04	0.84722715E-05
0.16872000E+04	0.87498347E-05
0.17249000E+04	0.89536497E-05
0.17618000E+04	0.90782105E-05
0.17988000E+04	0.92257196E-05
0.18728000E+04	0.96827825E-05
0.19473000E+04	0.10303558E-04
0.19843000E+04	0.10447263E-04
0.20583000E+04	0.10739693E-04
0.20953000E+04	0.10914401E-04
0.21323000E+04	0.11142944E-04
0.21693000E+04	0.11455126E-04
0.22068000E+04	0.11608087E-04
0.22438000E+04	0.11912422E-04
0.22808000E+04	0.11994993E-04
0.23178000E+04	0.12078134E-04
0.23548000E+04	0.12217990E-04
0.23918000E+04	0.12387964E-04
0.24295000E+04	0.12676524E-04
0.24665000E+04	0.12941953E-04
0.25405000E+04	0.13335213E-04
0.25775000E+04	0.13427644E-04
0.27260000E+04	0.13867565E-04
0.27630000E+04	0.14060461E-04
0.28370000E+04	0.14689257E-04
0.28740000E+04	0.14859348E-04
0.29110000E+04	0.15066068E-04
0.29487000E+04	0.15170511E-04
0.29857000E+04	0.15240523E-04
0.30227000E+04	0.15310872E-04
0.30597000E+04	0.15417012E-04
0.30967000E+04	0.15488150E-04
0.31337000E+04	0.15703628E-04
0.31713999E+04	0.15922093E-04
0.32083999E+04	0.16180506E-04
0.32453999E+04	0.16368167E-04
0.33193999E+04	0.16749425E-04
0.33563999E+04	0.16982440E-04
0.33933999E+04	0.16943372E-04
0.34675999E+04	0.17100136E-04
0.35048999E+04	0.17139550E-04
0.35418999E+04	0.17258360E-04
0.36158999E+04	0.17619748E-04
0.36535000E+04	0.17523795E-04
0.37275000E+04	0.18197010E-04
0.37645000E+04	0.18197013E-04
0.38015000E+04	0.18281007E-04
0.38385000E+04	0.18450168E-04
0.38755000E+04	0.18793169E-04
0.39131001E+04	0.19010780E 04
0.39501001E+04	0.18961046E-04
0.39871001E+04	0.1883[illegible]E-04
0.40611001E+04	0.192309[illegible]1E-04
0.40981001E+04	0.19498445E-04
0.41357998E+04	0.19633617E-04
0.41727998E+04	0.19724224E-04
0.42467998E+04	0.19678963E-04
0.42837998E+04	0.19815270E-04
0.43207998E+04	0.19998624E-04
0.43577998E+04	0.20090916E-04
0.44693999E+04	0.20606310E-04
0.45063999E+04	0.20558906E-04
0.45433999E+04	0.20511612E-04
0.45803999E+04	0.20558906E-04
0.46178999E+04	0.20844893E-04
0.46548999E+04	0.21134887E-04
0.46918999E+04	0.21379614E-04
0.47288999E+04	0.21476299E-04
0.48028999E+04	0.21476299E-04
0.48398999E+04	0.21577442E-04
0.48776001E+04	0.21577442E-04
0.49146001E+04	0.21577442E-04
0.49516001E+04	0.21727003E-04
0.50256001E+04	0.22029264E-04
0.50626001E+04	0.22335709E-04
0.51371001E+04	0.22284346E-04
0.51741001E+04	0.22284345E-04
0.52111001E+04	0.22335709E-04
0.52851001E+04	0.22803408E-04
0.53221001E+04	0.22961489E-04
0.53596001E+04	0.22803408E-04
0.53966001E+04	0.22855997E-04
0.54336001E+04	0.22961489E-04

Table B-1 (continued)

(a) Cell One

Time (sec)	[H^+] (M)	Time (sec)	[H^+] (M)
0.54706001E+04	0.23280923E-04	0.83454004E+04	0.27289763E-04
0.55446001E+04	0.23442271E-04	0.83824004E+04	0.27542281E-04
0.55816001E+04	0.23173932E-04	0.84194004E+04	0.27669414E-04
0.56192998E+04	0.23334582E-04	0.84564004E+04	0.27797107E-04
0.56562998E+04	0.23768394E-04	0.84934004E+04	0.27733186E-04
0.56932998E+04	0.23933164E-04	0.85307998E+04	0.27542281E-04
0.57302998E+04	0.23659208E-04	0.86047998E+04	0.27478945E-04
0.58417998E+04	0.24154599E-04	0.86417998E+04	0.27669414E-04
0.58787998E+04	0.24266117E-04	0.87157998E+04	0.27861226E-04
0.59157998E+04	0.24210271E-04	0.87527998E+04	0.27989805E-04
0.59527998E+04	0.24043638E-04	0.87905000E+04	0.27989805E-04
0.59897998E+04	0.24154599E-04	0.88275000E+04	0.27989805E-04
0.60267998E+04	0.24266117E-04	0.88645000E+04	0.27861226E-04
0.61013999E+04	0.24603654E-04	0.89015000E+04	0.27797107E-04
0.61383999E+04	0.24378103E-04	0.89755000E+04	0.27797107E-04
0.61753999E+04	0.24490631E-04	0.90130000E+04	0.27925442E-04
0.62123999E+04	0.24603654E-04	0.90500000E+04	0.28119004E-04
0.62863999E+04	0.25061106E-04	0.90870000E+04	0.28313934E-04
0.63241001E+04	0.24831315E-04	0.91240000E+04	0.28313934E-04
0.63611001E+04	0.24774215E-04	0.91610000E+04	0.28248798E-04
0.63981001E+04	0.24774215E-04	0.91980000E+04	0.28054315E-04
0.64351001E+04	0.24945934E-04	0.92542002E+04	0.28054315E-04
0.64721001E+04	0.25234791E-04	0.92912002E+04	0.27989805E-04
0.65461001E+04	0.25351272E-04	0.93282002E+04	0.28054315E-04
0.66206001E+04	0.25292977E-04	0.94390996E+04	0.28379192E-04
0.66576001E+04	0.25468316E-04	0.94760996E+04	0.28444601E-04
0.66946001E+04	0.25763196E-04	0.95137998E+04	0.28313934E-04
0.67316001E+04	0.25644822E-04	0.95507998E+04	0.28248798E-04
0.67686001E+04	0.25527015E-04	0.95877998E+04	0.28183813E-04
0.68056001E+04	0.25527015E-04	0.96247002E+04	0.28183813E-04
0.68432998E+04	0.25527015E-04	0.96617002E+04	0.28054315E-04
0.69172002E+04	0.25941796E-04	0.97364004E+04	0.28248798E-04
0.69542002E+04	0.26061514E-04	0.97734004E+04	0.28510161E-04
0.70282002E+04	0.25822599E-04	0.98104004E+04	0.28575900E-04
0.70658999E+04	0.25703954E-04	0.98474004E+04	0.28575900E-04
0.71028999E+04	0.25882142E-04	0.98844004E+04	0.28641762E-04
0.71398999E+04	0.26121606E-04	0.99214004E+04	0.28707804E-04
0.71768999E+04	0.26363314E-04	0.99584004E+04	0.28707804E-04
0.72508999E+04	0.26242182E-04	0.99960000E+04	0.28707804E-04
0.72878999E+04	0.26121606E-04	0.10033000E+05	0.28575900E-04
0.73256001E+04	0.26242182E-04	0.10070000E+05	0.28641762E-04
0.73996001E+04	0.26607257E-04	0.10144000E+05	0.28379192E-04
0.74366001E+04	0.26668582E-04	0.10219000E+05	0.28444601E-04
0.74736001E+04	0.26546048E-04	0.10256000E+05	0.28444601E-04
0.75106001E+04	0.26484979E-04	0.10293000E+05	0.28575900E-04
0.75482002E+04	0.26363314E-04	0.10330000E+05	0.28773997E-04
0.76037002E+04	0.26668582E-04	0.10367000E+05	0.28773997E-04
0.76407002E+04	0.26853431E-04	0.10404000E+05	0.28906787E-04
0.76777002E+04	0.27039589E-04	0.10478000E+05	0.28906787E-04
0.77892002E+04	0.26791682E-04	0.10515000E+05	0.28773997E-04
0.78262002E+04	0.26853431E-04	0.10552000E+05	0.28707804E-04
0.78632002E+04	0.27039589E-04	0.10589000E+05	0.28707804E-04
0.79002002E+04	0.27289763E-04	0.10626000E+05	0.28707804E-04
0.79742002E+04	0.27101911E-04	0.10663000E+05	0.28641762E-04
0.80112002E+04	0.26977412E-04	0.10700000E+05	0.28773997E-04
0.80488999E+04	0.26915324E-04	0.10738000E+05	0.28840315E-04
0.81043999E+04	0.27415757E-04	0.10775000E+05	0.28840315E-04
0.81413999E+04	0.27478945E-04	0.10849000E+05	0.29107179E-04
0.82154004E+04	0.27289763E-04	0.10886000E+05	0.29107179E-04
0.82714004E+04	0.27227010E-04	0.10923000E+05	0.29174265E-04
0.83084004E+04	0.27164402E-04	0.10997000E+05	0.29241535E-04

Table B-1 (continued)

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.11034000E+05	0.29040219E-04
0.11071000E+05	0.29040219E-04
0.11108000E+05	0.29040219E-04
0.11145000E+05	0.29040219E-04
0.11220000E+05	0.28906787E-04
0.11257000E+05	0.28906787E-04
0.11294000E+05	0.28840315E-04
0.11331000E+05	0.28906787E-04
0.11368000E+05	0.29040219E-04
0.11405000E+05	0.28973413E-04
0.11461000E+05	0.29107179E-04
0.11498000E+05	0.29308932E-04
0.11572000E+05	0.29308932E-04
0.11609000E+05	0.29376484E-04
0.11646000E+05	0.29444191E-04
0.11684000E+05	0.29376484E-04
0.11721000E+05	0.29376484E-04
0.11795000E+05	0.29444191E-04
0.11832000E+05	0.29512083E-04
0.11869000E+05	0.29444191E-04
0.11906000E+05	0.29444191E-04
0.11980000E+05	0.29376484E-04
0.12017000E+05	0.29376484E-04
0.12054000E+05	0.29376484E-04
0.12091000E+05	0.29376484E-04
0.12128000E+05	0.29376484E-04
0.12166000E+05	0.29174265E-04
0.12203000E+05	0.29174265E-04
0.12277000E+05	0.29174265E-04
0.12314000E+05	0.29308932E-04
0.12351000E+05	0.29241535E-04
0.12388000E+05	0.29241535E-04
0.12425000E+05	0.29174265E-04
0.12462000E+05	0.29308932E-04
0.12499000E+05	0.29308932E-04
0.12573000E+05	0.29308932E-04
0.12610000E+05	0.29376484E-04
0.12647000E+05	0.29376484E-04
0.12722000E+05	0.29580131E-04
0.12759000E+05	0.29580131E-04
0.12796000E+05	0.29580131E-04
0.12833000E+05	0.29648309E-04
0.12870000E+05	0.29785162E-04
0.12908000E+05	0.29648309E-04
0.12952000E+05	0.29785162E-04
0.13019000E+05	0.29853813E-04
0.13056000E+05	0.29853813E-04
0.13111000E+05	0.29853813E-04
0.13149000E+05	0.29922619E-04
0.13186000E+05	0.29853813E-04
0.13223000E+05	0.29853813E-04
0.13260000E+05	0.29853813E-04

Table B-1 (continued)

(b) Cell Two

Time (sec)	$[H^+]$ (M)	Time (sec)	$[H^+]$ (M)
0.20170000E+02	0.96161195E-07	0.11510000E+04	0.77624654E-05
0.38669998E+02	0.93972332E-07	0.11695000E+04	0.78704552E-05
0.57160000E+02	0.[illegible]933115E-07	0.12812000E+04	0.89742862E-05
0.75669996E+02	0.91621942E-07	0.12997000E+04	0.91411266E-05
0.94160004E+02	0.84527690E-07	0.13367000E+04	0.95939986E-05
0.11266000E+03	0.84333514E-07	0.13552000E+04	0.98174778E-05
0.13114999E+03	0.10592531E-06	0.13737000E+04	0.10069309E-04
0.14964999E+03	0.15452544E-06	0.13922000E+04	0.10232930E-04
0.16814999E+03	0.18578046E-06	0.14292000E+04	0.10566174E-04
0.18664999E+03	0.20511609E-06	0.14480000E+04	0.10715195E-04
0.20514000E+03	0.21426859E-06	0.14667000E+04	0.10864253E-04
0.22394000E+03	0.23227365E-06	0.14852000E+04	0.11015353E-04
0.24264000E+03	0.24774212E-06	0.15222000E+04	0.11455126E-04
0.26114001E+03	0.28313931E-06	0.15407000E+04	0.11830411E-04
0.27964001E+03	0.31768730E-06	0.15592000E+04	0.11939879E-04
0.29813000E+03	0.34593924E-06	0.15777000E+04	0.12246151E-04
0.31663000E+03	0.37757221E-06	0.16147000E+04	0.12618268E-04
0.33513000E+03	0.40271695E-06	0.16332000E+04	0.12764390E-04
0.35363000E+03	0.43751396E-06	0.16702000E+04	0.13001692E-04
0.37213000E+03	0.47315140E-06	0.17263000E+04	0.13583127E-04
0.39062000E+03	0.53210763E-06	0.17818000E+04	0.14092894E-04
0.40912000E+03	0.59292512E-06	0.18003000E+04	0.14354894E-04
0.42762000E+03	0.64853423E-06	0.18373000E+04	0.14859348E-04
0.44611999E+03	0.71779397E-06	0.18556000E+04	0.14996844E-04
0.46497000E+03	0.79983351E-06	0.18743000E+04	0.15240523E-04
0.48378000E+03	0.86696173E-06	0.18928000E+04	0.15381531E-04
0.50228000E+03	0.97723648E-06	0.19301000E+04	0.15417012E-04
0.52077002E+03	0.10914406E-05	0.19488000E+04	0.15595515E-04
0.53927002E+03	0.12022643E-05	0.19673000E+04	0.15812475E-04
0.55777002E+03	0.13304542E-05	0.19858000E+04	0.15922093E-04
0.57627002E+03	0.14689250E-05	0.20228000E+04	0.16519609E-04
0.59476001E+03	0.16180798E-05	0.20413000E+04	0.16557698E-04
0.61326001E+03	0.17782793E-05	0.20598000E+04	0.16904411E-04
0.63176001E+03	0.19453601E-05	0.21338000E+04	0.17660392E-04
0.65025000E+03	0.21232454E-05	0.21523000E+04	0.17664870E-04
0.66875000E+03	0.22961473E-05	0.22083000E+04	0.18071731E-04
0.68725000E+03	0.24886559E-05	0.22638000E+04	0.18365372E-04
0.70616998E+03	0.26791663E-05	0.22823000E+04	0.18706520E-04
0.72490997E+03	0.28575865E-05	0.23378000E+04	0.19166689E-04
0.74340002E+03	0.30760948E-05	0.23748000E+04	0.19769686E-04
0.76190002E+03	0.32734056E-05	0.23933000E+04	0.19860941E-04
0.78040002E+03	0.34673674E-05	0.24122000E+04	0.20090916E-04
0.79890002E+03	0.36728222E-05	0.24310000E+04	0.20417367E-04
0.81740002E+03	0.38636607E-05	0.24495000E+04	0.20230193E-04
0.83589001E+03	0.40831928E-05	0.25420000E+04	0.20749121E-04
0.85439001E+03	0.42854836E-05	0.25790000E+04	0.20592961E-04
0.87290002E+03	0.44374532E-05	0.26160000E+04	0.21281401E-04
0.89139001E+03	0.47097719E-05	0.26345000E+04	0.21428890E-04
0.90988000E+03	0.48752859E-05	0.26533000E+04	0.21577442E-04
0.92838000E+03	0.50933036E-05	0.27630000E+04	0.22961489E-04
0.94688000E+03	0.52844525E-05	0.28015000E+04	0.23014412E-04
0.96567999E+03	0.55080777E-05	0.28200000E+04	0.23014412E-04
0.98454999E+03	0.57147872E-05	0.28940000E+04	0.23173932E-04
0.10030000E+04	0.58884339E-05	0.29128000E+04	0.23659208E-04
0.10215000E+04	0.61376181E-05	0.29687000E+04	0.23768394E-04
0.10400000E+04	0.63386942E-05	0.30242000E+04	0.24547078E-04
0.10585000E+04	0.65014527E-05	0.30612000E+04	0.24774215E-04
0.10770000E+04	0.67142864E-05	0.30797000E+04	0.25003430E-04
0.10955000E+04	0.69024009E-05	0.31541001E+04	0.25468316E-04
0.11140000E+04	0.73451433E-05	0.32468000E+04	0.25822599E-04
0.11325000E+04	0.77803643E-05	0.32653000E+04	0.26121605E-04

Table B-1 (continued)

(b) Cell Two

Time (sec)	$[H^+]$ (M)	Time (sec)	$[H^+]$ (M)
0.32836000E+04	0.26181839E-04	0.60656001E+04	0.38547042E-04
0.33023000E+04	0.26242182E-04	0.60843999E+04	0.37931506E-04
0.33578000E+04	0.26668582E-04	0.61028999E+04	0.38194386E-04
0.33951001E+04	0.27039589E-04	0.61213999E+04	0.38459162E-04
0.34138000E+04	0.26853431E-04	0.61765999E+04	0.38994196E-04
0.34323000E+04	0.26915324E-04	0.62508999E+04	0.38725739E-04
0.35803000E+04	0.28054315E-04	0.63067998E+04	0.38547842E-04
0.36550000E+04	0.28379192E-04	0.63256001E+04	0.38815069E-04
0.36735000E+04	0.28379192E-04	0.63441001E+04	0.38725739E-04
0.36920000E+04	0.28510161E-04	0.63626001E+04	0.39445763E-04
0.37475000E+04	0.28840315E-04	0.63811001E+04	0.39084072E-04
0.37660000E+04	0.29174265E-04	0.64921001E+04	0.39174192E-04
0.37845000E+04	0.29241535E-04	0.65106001E+04	0.38994196E-04
0.38961001E+04	0.29648309E-04	0.65663999E+04	0.39994484E-04
0.39886001E+04	0.30130053E-04	0.66036001E+04	0.39536677E-04
0.40071001E+04	0.30549214E-04	0.66591001E+04	0.39536677E-04
0.40441001E+04	0.30760963E-04	0.67146001E+04	0.39536677E-04
0.40626001E+04	0.30549214E-04	0.67331001E+04	0.39536677E-04
0.41557998E+04	0.31117153E-04	0.67516001E+04	0.39902476E-04
0.41742996E+04	0.30902924E-04	0.68073999E+04	0.40086699E-04
0.41927998E+04	0.31188902E-04	0.68632002E+04	0.40550336E-04
0.42112996E+04	0.31117153E-04	0.68817002E+04	0.39994494E-04
0.43037998E+04	0.31988966E-04	0.69002002E+04	0.40271698E-04
0.43222998E+04	0.32284930E-04	0.69557002E+04	0.40179093E-04
0.43407998E+04	0.32508742E-04	0.69927002E+04	0.39994484E-04
0.44153999E+04	0.32210661E-04	0.70112002E+04	0.40364517E-04
0.44338999E+04	0.32433956E-04	0.70858999E+04	0.41209732E-04
0.45448999E+04	0.32960965E-04	0.71413999E+04	0.40738018E-04
0.45633999E+04	0.33419510E-04	0.71598999E+04	0.40738018E-04
0.45818999E+04	0.33189430E-04	0.71783999E+04	0.40831950E-04
0.46563999E+04	0.33496533E-04	0.72153999E+04	0.40926061E-04
0.47488999E+04	0.33419510E-04	0.72523999E+04	0.41304753E-04
0.47673999E+04	0.33419510E-04	0.72897002E+04	0.41020387E-04
0.47858999E+04	0.33806449E-04	0.73085000E+04	0.41114970E-04
0.48043999E+04	0.33651151E-04	0.73270000E+04	0.41495412E-04
0.48228999E+04	0.33884433E-04	0.73455000E+04	0.41399955E-04
0.48413999E+04	0.34514374E-04	0.74750000E+04	0.41114970E-04
0.50086001E+04	0.35399709E-04	0.74935000E+04	0.41304753E-04
0.50271001E+04	0.34994533E-04	0.75120000E+04	0.41495412E-04
0.50826001E+04	0.34753606E-04	0.75497002E+04	0.41399955E-04
0.51386001E+04	0.35237092E-04	0.75682002E+04	0.41975902E-04
0.51571001E+04	0.35809648E-04	0.76052002E+04	0.42266849E-04
0.51756001E+04	0.35563146E-04	0.76237002E+04	0.41685912E-04
0.52311001E+04	0.35809648E-04	0.76422002E+04	0.41685912E-04
0.52496001E+04	0.36057856E-04	0.76977002E+04	0.41304753E-04
0.53423999E+04	0.35727269E-04	0.77162002E+04	0.41685912E-04
0.53611001E+04	0.35892182E-04	0.77720000E+04	0.41975902E-04
0.54166001E+04	0.36475380E-04	0.77907002E+04	0.41975902E-04
0.54721001E+04	0.36475380E-04	0.78832002E+04	0.41782994E-04
0.55646001E+04	0.36559486E-04	0.79202002E+04	0.41685912E-04
0.55835000E+04	0.37068057E-04	0.79757002E+04	0.41975902E-04
0.56022002E+04	0.36897738E-04	0.80130000E+04	0.42072646E-04
0.56207002E+04	0.37153528E-04	0.80317998E+04	0.42364267E-04
0.56947002E+04	0.37239159E-04	0.80502998E+04	0.41975902E-04
0.57132002E+04	0.36897738E-04	0.80687998E+04	0.42169657E-04
0.58057002E+04	0.37497277E-04	0.81427998E+04	0.41879375E-04
0.58245000E+04	0.37497277E-04	0.81612998E+04	0.42072644E-04
0.58432002E+04	0.37583701E-04	0.81797998E+04	0.41495412E-04
0.58987002E+04	0.37411053E-04	0.81982996E+04	0.41975902E-04
0.59172002E+04	0.37583701E-04	0.82540996E+04	0.42266849E-04
0.60467002E+04	0.38016930E-04	0.84022998E+04	0.42461910E-04

Table B-1 (concluded)

(b) Cell Two

Time (sec)	$[H^+]$ (M)
0.84207998E+04	0.42657950E-04
0.84947998E+04	0.42072644E-04
0.85135996E+04	0.42854856E-04
0.85322998E+04	0.42559659E-04
0.85507996E+04	0.42559659E-04
0.86432998E+04	0.43151940E-04
0.86617998E+04	0.43451000E-04
0.87172996E+04	0.42756270E-04
0.87357998E+04	0.43052631E-04
0.87920000E+04	0.42657950E-04
0.89030000E+04	0.43251399E-04
0.89215000E+04	0.43251399E-04
0.89400000E+04	0.43151940E-04
0.89957996E+04	0.43551190E-04
0.90145000E+04	0.42953630E-04
0.90330000E+04	0.42756270E-04
0.90885000E+04	0.42756270E-04
0.91624004E+04	0.42461910E-04
0.91809004E+04	0.42559659E-04
0.91994004E+04	0.42559659E-04
0.92179004E+04	0.42953630E-04
0.92367998E+04	0.43551190E-04
0.93110996E+04	0.43752176E-04
0.94730000E+04	0.43351057E-04
0.94967002E+04	0.43551190E-04
0.95152002E+04	0.43052631E-04
0.96262002E+04	0.43752178E-04
0.96447002E+04	0.43551190E-04
0.96632002E+04	0.43752173E-04
0.97190000E+04	0.43451000E-04
0.97379004E+04	0.43954176E-04
0.97564004E+04	0.43752173E-04
0.97934004E+04	0.43752173E-04
0.98117998E+04	0.43651569E-04
0.98672998E+04	0.43251399E-04
0.98857996E+04	0.43151940E-04
0.10016000E+05	0.44055483E-04

Table B-2

Data for Mustard Hydrolysis at 288 K

(a) Cell One

Time (sec)	$[H^+]$ (M)	Time (sec)	$[H^+]$ (M)
0.18700001E+02	0.19860940E-06	0.22806001E+04	0.42461910E-04
0.55689999E+02	0.30130050E-06	0.23176001E+04	0.42756270E-04
0.92680000E+02	0.39174188E-06	0.23546001E+04	0.43551190E-04
0.12967999E+03	0.56754459E-06	0.23916001E+04	0.43954176E-04
0.16667000E+03	0.74130980E-06	0.24292000E+04	0.44157323E-04
0.20366000E+03	0.11015368E-05	0.24662000E+04	0.44771365E-04
0.24114000E+03	0.14893603E-05	0.25032000E+04	0.45239783E-04
0.27813000E+03	0.21627184E-05	0.25402000E+04	0.45394172E-04
0.31513000E+03	0.28183824E-05	0.25772000E+04	0.45814166E-04
0.35212000E+03	0.37583720E-05	0.26142000E+04	0.46451521E-04
0.38910999E+03	0.45394149E-05	0.26512000E+04	0.46558031E-04
0.42610001E+03	0.56234144E-05	0.26883999E+04	0.46773494E-04
0.46307999E+03	0.63526301E-05	0.27258999E+04	0.47424197E-04
0.50073999E+03	0.74644922E-05	0.27628999E+04	0.47533500E-04
0.53772998E+03	0.83560244E-05	0.27998999E+04	0.47752910E-04
0.57471997E+03	0.93540565E-05	0.28368000E+04	0.48194775E-04
0.61171002E+03	0.10303558E-04	0.28738000E+04	0.48640683E-04
0.64870001E+03	0.11246051E-04	0.29108000E+04	0.48528833E-04
0.68569000E+03	0.12105964E-04	0.29485000E+04	0.49431026E-04
0.72334998E+03	0.13091824E-04	0.29855000E+04	0.49431026E-04
0.76034003E+03	0.14028128E-04	0.30225000E+04	0.49431026E-04
0.79733002E+03	0.14927958E-04	0.30595000E+04	0.50118699E-04
0.83432001E+03	0.15776115E-04	0.30965000E+04	0.50350392E-04
0.87131000E+03	0.16672468E-04	0.31335000E+04	0.50234263E-04
0.90829999E+03	0.17418075E-04	0.31711001E+04	0.50933060E-04
0.94529999E+03	0.18407720E-04	0.32081001E+04	0.51050501E-04
0.98296002E+03	0.19142552E-04	0.32451001E+04	0.51050501E-04
0.10200000E+04	0.20090916E-04	0.32821001E+04	0.51641629E-04
0.10569000E+04	0.20844698E-04	0.33191001E+04	0.51880004E-04
0.10939000E+04	0.21627175E-04	0.33561001E+04	0.51880004E-04
0.11309000E+04	0.22490547E-04	0.33931001E+04	0.52360007E-04
0.11679000E+04	0.23227367E-04	0.34308000E+04	0.52480736E-04
0.12049000E+04	0.24043532E-04	0.34678000E+04	0.52601747E-04
0.12426000E+04	0.24774215E-04	0.35048000E+04	0.53210784E-04
0.12796000E+04	0.25585850E-04	0.35417000E+04	0.53038424E-04
0.13166000E+04	0.26363314E-04	0.35787000E+04	0.53210784E-04
0.13536000E+04	0.27101911E-04	0.36157000E+04	0.53326978E-04
0.13906000E+04	0.27861226E-04	0.36532000E+04	0.53703152E-04
0.14276000E+04	0.28575900E-04	0.36902000E+04	0.54075386E-04
0.14652000E+04	0.29376484E-04	0.37272000E+04	0.54325046E-04
0.15022000E+04	0.30060768E-04	0.37642000E+04	0.54200125E-04
0.15392000E+04	0.30690229E-04	0.38012000E+04	0.54827673E-04
0.15762000E+04	0.31332838E-04	0.38382000E+04	0.54575754E-04
0.16132000E+04	0.31988966E-04	0.38752000E+04	0.54827673E-04
0.16502000E+04	0.32734042E-04	0.39123999E+04	0.55207754E-04
0.16872000E+04	0.33419510E-04	0.39495999E+04	0.54627673E-04
0.17247000E+04	0.34040809E-04	0.39863999E+04	0.55975794E-04
0.17617000E+04	0.34673692E-04	0.40233999E+04	0.55462337E-04
0.17987000E+04	0.35399709E-04	0.40605999E+04	0.55847020E-04
0.18357000E+04	0.35974939E-04	0.40976999E+04	0.56234119E-04
0.18727000E+04	0.36475380E-04	0.41355000E+04	0.55347020E-04
0.19096000E+04	0.37155528E-04	0.41725000E+04	0.56885325E-04
0.19471000E+04	0.37757221E-04	0.42095000E+04	0.56104607E-04
0.19841000E+04	0.38144388E-04	0.42465000E+04	0.56623900E-04
0.20211000E+04	0.38904531E-04	0.42835000E+04	0.57544014E-04
0.20581001E+04	0.39354978E-04	0.43205000E+04	0.56623900E-04
0.20951001E+04	0.39719136E-04	0.43575000E+04	0.57147849E-04
0.21321001E+04	0.40457591E-04	0.43952002E+04	0.57544014E-04
0.21691001E+04	0.40926061E-04	0.44322002E+04	0.56885325E-04
0.22066001E+04	0.41304753E-04	0.44692002E+04	0.57942874E-04
0.22436001E+04	0.42072048E-04	0.45062002E+04	0.57942874E-04

Table B-2 (continued)

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.45432002E+04	0.57279562E-04
0.45802002E+04	0.58210277E-04
0.46177998E+04	0.58070421E-04
0.46547998E+04	0.57411635E-04
0.46917998E+04	0.58070421E-04
0.47287998E+04	0.58748963E-04
0.47657998E+04	0.57809633E-04
0.48027998E+04	0.57942874E-04
0.48397998E+04	0.58884369E-04
0.48772998E+04	0.58479029E-04
0.49142998E+04	0.57942874E-04
0.49512998E+04	0.58884369E-04
0.49882998E+04	0.59156115E-04
0.50252998E+04	0.58479029E-04
0.50622998E+04	0.58884369E-04
0.50992998E+04	0.59566206E-04
0.51367998E+04	0.58613812E-04
0.51737998E+04	0.59292517E-04
0.52107998E+04	0.59429232E-04
0.52477998E+04	0.58884369E-04
0.52847998E+04	0.59429232E-04
0.53217998E+04	0.59979030E-04
0.53592998E+04	0.59292517E-04
0.53962998E+04	0.59703554E-04
0.54332998E+04	0.60255996E-04
0.54702998E+04	0.59566206E-04
0.55072998E+04	0.59429232E-04
0.55442998E+04	0.60394876E-04
0.55812998E+04	0.59429232E-04
0.56190000E+04	0.59979080E-04
0.56560000E+04	0.60394876E-04
0.56930000E+04	0.59841157E-04
0.57300000E+04	0.60313498E-04
0.57670000E+04	0.60673596E-04
0.58040000E+04	0.60255996E-04
0.58417002E+04	0.61094150E-04
0.58787002E+04	0.60255996E-04
0.59157002E+04	0.60953662E-04
0.59527002E+04	0.61235078E-04
0.59897002E+04	0.60394876E-04
0.60266001E+04	0.61517676E-04
0.60636001E+04	0.61094150E-04
0.61012998E+04	0.61094150E-04
0.61382998E+04	0.61801635E-04
0.61752998E+04	0.60953662E-04
0.62122998E+04	0.61659463E-04
0.62492998E+04	0.61376209E-04
0.62862998E+04	0.61235078E-04
0.63237998E+04	0.62086903E-04
0.63607998E+04	0.61376209E-04
0.63977998E+04	0.61659463E-04
0.64347998E+04	0.62373489E-04
0.64717998E+04	0.61801635E-04
0.65087998E+04	0.61376209E-04
0.65457998E+04	0.62373489E-04
0.65832998E+04	0.62230065E-04
0.66202998E+04	0.61801635E-04
0.66572002E+04	0.62230065E-04
0.66942002E+04	0.62805826E-04
0.67312002E+04	0.62086903E-04
0.67682002E+04	0.61659463E-04

Time (sec)	$[H^+]$ (M)
0.68052002E+04	0.62086903E-04
0.68428999E+04	0.62950581E-04
0.68798999E+04	0.62230065E-04
0.69168999E+04	0.61944076E-04
0.69538999E+04	0.62805826E-04
0.69908999E+04	0.63095729E-04
0.70278999E+04	0.62230065E-04
0.70655000E+04	0.62230065E-04
0.71025000E+04	0.63095729E-04
0.71395000E+04	0.62805826E-04
0.71765000E+04	0.62086903E-04
0.72135000E+04	0.62661340E-04
0.72505000E+04	0.63386979E-04
0.72875000E+04	0.63095729E-04
0.73250000E+04	0.62373489E-04
0.73620000E+04	0.62805826E-04
0.73990000E+04	0.63386979E-04
0.74360000E+04	0.63679505E-04
0.74730000E+04	0.62950581E-04
0.75285000E+04	0.62805826E-04
0.75660000E+04	0.63533073E-04
0.76035000E+04	0.63826337E-04
0.76400000E+04	0.63241219E-04
0.76770000E+04	0.62661340E-04
0.77140000E+04	0.62950581E-04
0.77510000E+04	0.62950581E-04
0.77887002E+04	0.63826337E-04
0.78257002E+04	0.63973505E-04
0.78627002E+04	0.63826337E-04
0.78997002E+04	0.63095729E-04
0.79367002E+04	0.63241219E-04
0.79737002E+04	0.63533073E-04
0.80107002E+04	0.64120955E-04
0.80482998E+04	0.64120955E-04
0.80852998E+04	0.63679508E-04
0.81222998E+04	0.63386979E-04
0.81592998E+04	0.63533073E-04
0.81962998E+04	0.63826337E-04
0.82332998E+04	0.64416927E-04
0.82709004E+04	0.64565400E-04
0.83079004E+04	0.63826337E-04
0.83449004E+04	0.63679508E-04
0.83819004E+04	0.63826337E-04
0.84189004E+04	0.63679508E-04
0.84559004E+04	0.63826337E-04
0.84929004E+04	0.64565400E-04
0.85304004E+04	0.64714208E-04
0.85674004E+04	0.63973505E-04
0.86044004E+04	0.63533073E-04
0.86414004E+04	0.63386979E-04
0.86784004E+04	0.63679508E-04
0.87154004E+04	0.64120955E-04
0.87524004E+04	0.64416927E-04
0.87900000E+04	0.64565400E-04
0.88270000E+04	0.63973505E-04
0.88640000E+04	0.63679508E-04
0.89010000E+04	0.63826337E-04
0.89380000E+04	0.64565400E-04

Table B-2 (continued)

(b) Cell Two

Time (sec)	$[H^+]$ (M)	Time (sec)	$[H^+]$ (M)
0.20160000E+02	0.72110758E-07	0.11509000E+04	0.30902922E-06
0.38660000E+02	0.74130945E-07	0.11694000E+04	0.31477495E-06
0.57150002E+02	0.72443541E-07	0.12255000E+04	0.33419509E-06
0.75650002E+02	0.70307294E-07	0.12440000E+04	0.34355759E-06
0.94139999E+02	0.72110758E-07	0.12625000E+04	0.35156029E-06
0.11265000E+03	0.81470354E-07	0.12995000E+04	0.36728238E-06
0.13114000E+03	0.85703739E-07	0.13180000E+04	0.37670395E-06
0.14964000E+03	0.85310035E-07	0.13365000E+04	0.38370723E-06
0.16813000E+03	0.86496769E-07	0.13920000E+04	0.40457587E-06
0.18663000E+03	0.90573174E-07	0.14290000E+04	0.41879372E-06
0.20513000E+03	0.92896656E-07	0.14479000E+04	0.43052628E-06
0.22361000E+03	0.99770070E-07	0.14667000E+04	0.43752175E-06
0.24261000E+03	0.99770070E-07	0.14852000E+04	0.44977980E-06
0.26110999E+03	0.10423179E-06	0.15222000E+04	0.46881343E-06
0.27960001E+03	0.10519606E-06	0.15592000E+04	0.48065240E-06
0.29810001E+03	0.10592531E-06	0.15777000E+04	0.49388416E-06
0.31659000E+03	0.11142943E-06	0.16147000E+04	0.51286145E-06
0.33509000E+03	0.11508001E-06	0.16332000E+04	0.51679999E-06
0.35357999E+03	0.11587778E-06	0.16516000E+04	0.53333525E-06
0.37207999E+03	0.11534524E-06	0.16889000E+04	0.55975769E-06
0.39057001E+03	0.12022637E-06	0.17261000E+04	0.58613807E-06
0.40907001E+03	0.12559251E-06	0.17446000E+04	0.59841153E-06
0.42756000E+03	0.12502591E-06	0.17816000E+04	0.62517[illegible]0E-06
0.44606000E+03	0.12502591E-06	0.18186000E+04	0.65313[illegible]77E-06
0.46492001E+03	0.13031658E-06	0.18371000E+04	0.66527309E-06
0.48370999E+03	0.13772092E-06	0.19111000E+04	0.72110726E-06
0.50220001E+03	0.13772092E-06	0.19299000E+04	0.74130980E-06
0.52070001E+03	0.14286950E-06	0.20041000E+04	0.80909561E-06
0.53919000E+03	0.15066067E-06	0.20226000E+04	0.82224250E-06
0.55769000E+03	0.15346160E-06	0.20411000E+04	0.83368133E-06
0.57619000E+03	0.15417011E-06	0.20596001E+04	0.85113749E-06
0.59467999E+03	0.15958790E-06	0.20966001E+04	0.89125058E-06
0.61316998E+03	0.16405907E-06	0.21151001E+04	0.92045002E-06
0.63166998E+03	0.16595861E-06	0.21521001E+04	0.95499217E-06
0.65015997E+03	0.16943370E-06	0.21896001E+04	0.10046157E-05
0.66865997E+03	0.17458220E-06	0.22081001E+04	0.10280158E-05
0.68715002E+03	0.17988714E-06	0.22266001E+04	0.10543557E-05
0.70603996E+03	0.18407718E-06	0.22821001E+04	0.11142938E-05
0.72481000E+03	0.18793168E-06	0.23006001E+04	0.11428779E-05
0.74331000E+03	0.19453590E-06	0.23376001E+04	0.11830416E-05
0.76179999E+03	0.19998622E-06	0.23560000E+04	0.12133891E-05
0.78028998E+03	0.20844897E-06	0.23931001E+04	0.12735031E-05
0.79879999E+03	0.21281399E-06	0.24307000E+04	0.13243424E-05
0.81728003E+03	0.21727001E-06	0.24492000E+04	0.13614440E-05
0.83578003E+03	0.22284345E-06	0.24677000E+04	0.14060466E-05
0.85428003E+03	0.22855987E-06	0.25047000E+04	0.14825172E-05
0.87277002E+03	0.23120643E-06	0.25232000E+04	0.15170534E-05
0.89127002E+03	0.23659206E-06	0.25417000E+04	0.15631466E-05
0.90977002E+03	0.24266114E-06	0.25602000E+04	0.16120798E-05
0.92826001E+03	0.25003428E-06	0.26157000E+04	0.17377996E-05
0.94676001E+03	0.25468313E-06	0.26530000E+04	0.18030183E-05
0.96565997E+03	0.26242182E-06	0.26718000E+04	0.18492696E-05
0.98441996E+03	0.26484977E-06	0.27088000E+04	0.19453601E-05
0.10029000E+04	0.27039567E-06	0.27458000E+04	0.20370426E-05
0.10214000E+04	0.27605785E-06	0.27643000E+04	0.20592971E-05
0.10399000E+04	0.28119001E-06	0.27828000E+04	0.21478268E-05
0.10584000E+04	0.28510161E-06	0.28013000E+04	0.22080026E-05
0.10769000E+04	0.29107179E-06	0.28198000E+04	0.22594350E-05
0.10954000E+04	0.29241534E-06	0.28938000E+04	0.24717233E-05
0.11139000E+04	0.29853811E-06	0.29127000E+04	0.25234801E-05
0.11324000E+04	0.30478964E-06	0.29315000E+04	0.26242194E-05

Table B-2 (continued)

(b) Cell Two

Time (sec)	$[H^+]$ (M)
0.29670000E+04	0.28183824E-05
0.30055000E+04	0.29107191E-05
0.30240000E+04	0.29922633E-05
0.30425000E+04	0.30760948E-05
0.30793999E+04	0.32433970E-05
0.31348999E+04	0.34593941E-05
0.31538000E+04	0.35892162E-05
0.31726001E+04	0.36554502E-05
0.32096001E+04	0.37757238E-05
0.32281001E+04	0.39084029E-05
0.32466001E+04	0.40364534E-05
0.32651001E+04	0.41304770E-05
0.33391001E+04	0.44565631E-05
0.33576001E+04	0.45498219E-05
0.33761001E+04	0.46665959E-05
0.33950000E+04	0.47533522E-05
0.34507000E+04	0.50466115E-05
0.34692000E+04	0.51641605E-05
0.34877000E+04	0.53086447E-05
0.35062000E+04	0.53826952E-05
0.35617000E+04	0.57147872E-05
0.35802000E+04	0.58210303E-05
0.35987000E+04	0.59824339E-05
0.36172000E+04	0.59979106E-05
0.36360000E+04	0.61801602E-05
0.37102000E+04	0.65313047E-05
0.37287000E+04	0.65917338E-05
0.37657000E+04	0.68706800E-05
0.38212000E+04	0.70145556E-05
0.38397000E+04	0.71779432E-05
0.38582000E+04	0.73113879E-05
0.38770000E+04	0.73282395E-05
0.39143000E+04	0.74989402E-05
0.39328000E+04	0.76207880E-05
0.39698000E+04	0.78685951E-05
0.39883000E+04	0.81096105E-05
0.40433000E+04	0.83945952E-05
0.40623000E+04	0.83368095E-05
0.40808000E+04	0.84527392E-05
0.41182002E+04	0.86496775E-05
0.41555000E+04	0.88307979E-05
0.41925000E+04	0.89536497E-05
0.42110000E+04	0.90573176E-05
0.42295000E+04	0.92257196E-05
0.42480000E+04	0.93110775E-05
0.42850000E+04	0.92044957E-05
0.43035000E+04	0.93540566E-05
0.43781001E+04	0.96605072E-05
0.44151001E+04	0.99083109E-05
0.44336001E+04	0.10092534E-04
0.44521001E+04	0.10209389E-04
0.44706001E+04	0.10139112E-04
0.45076001E+04	0.10250164E-04
0.45261001E+04	0.10399301E-04
0.45631001E+04	0.10641426E-04
0.45816001E+04	0.10616955E-04
0.46377998E+04	0.10715195E-04
0.46562998E+04	0.10789467E-04
0.46747998E+04	0.10839260E-04
0.46932998E+04	0.10864253E-04
0.47487998E+04	0.10964781E-04
0.47857998E+04	0.11168627E-04
0.48042998E+04	0.11271972E-04
0.48412998E+04	0.11376273E-04
0.48787998E+04	0.11350102E-04
0.48972998E+04	0.11587778E-04
0.49527998E+04	0.11885018E-04
0.49712998E+04	0.11694990E-04
0.50452998E+04	0.12078134E-04
0.50822998E+04	0.12161864E-04
0.51011001E+04	0.12274400E-04
0.51197998E+04	0.12331045E-04
0.51567998E+04	0.12359477E-04
0.51752998E+04	0.12387964E-04
0.51937998E+04	0.12331045E-04
0.52122998E+04	0.12331045E-04
0.53047998E+04	0.12735026E-04
0.53232998E+04	0.12735026E-04
0.53607998E+04	0.13001692E-04
0.53792998E+04	0.13091824E-04
0.53977998E+04	0.13121999E-04
0.54347998E+04	0.13001692E-04
0.54902998E+04	0.13152242E-04
0.55087998E+04	0.13304549E-04
0.55272998E+04	0.13335213E-04
0.55832002E+04	0.13273941E-04
0.56020000E+04	0.13365949E-04
0.56205000E+04	0.13427644E-04
0.56945000E+04	0.13677290E-04
0.57130000E+04	0.13614434E-04
0.57315000E+04	0.13740423E-04
0.57870000E+04	0.13772092E-04
0.58055000E+04	0.13963686E-04
0.58431001E+04	0.13803834E-04
0.58801001E+04	0.13995870E-04
0.58986001E+04	0.14092894E-04
0.59171001E+04	0.14125376E-04
0.59356001E+04	0.13963686E-04
0.59726001E+04	0.14125376E-04
0.60466001E+04	0.14157932E-04
0.60842998E+04	0.14387980E-04
0.61027998E+04	0.14521113E-04
0.61397998E+04	0.14387980E-04
0.61582998E+04	0.14354894E-04
0.61952998E+04	0.14454393E-04
0.62877998E+04	0.14621764E-04
0.63065000E+04	0.14689257E-04
0.63252002E+04	0.14689257E-04
0.63437002E+04	0.14621764E-04
0.63807998E+04	0.14723128E-04
0.64177002E+04	0.14791088E-04
0.64362002E+04	0.14723128E-04
0.64547002E+04	0.14757062E-04
0.65287002E+04	0.15100793E-04
0.65472002E+04	0.15066068E-04
0.65660000E+04	0.14996844E-04
0.66032002E+04	0.14893611E-04
0.66217002E+04	0.14996844E-04
0.66402002E+04	0.15205476E-04
0.66587002E+04	0.15417012E-04
0.67882002E+04	0.15205476E-04
0.68070000E+04	0.15100793E-04

Table B-2 (concluded)

(b) Cell Two

Time (sec)	$[H^+]$ (M)
0.68442995E+04	0.15135597E-04
0.68997996E+04	0.15275604E-04
0.69182993E+04	0.15275664E-04
0.69367996E+04	0.15310872E-04
0.69552996E+04	0.15310872E-04
0.70482002E+04	0.15346161E-04
0.70670000E+04	0.15346161E-04
0.70855000E+04	0.15381531E-04
0.71040000E+04	0.15275604E-04
0.71225000E+04	0.15417012E-04
0.72705000E+04	0.15438160E-04
0.72892002E+04	0.15523372E-04
0.73060000E+04	0.15417012E-04
0.73635000E+04	0.15559652E-04
0.73320000E+04	0.15452544E-04
0.74190000E+04	0.15381531E-04
0.74930000E+04	0.15523372E-04
0.75675000E+04	0.15559652E-04
0.75860000E+04	0.15523372E-04
0.76045000E+04	0.15485160E-04
0.76970000E+04	0.15703628E-04
0.77155000E+04	0.15776115E-04
0.77340000E+04	0.15812475E-04
0.77901001E+04	0.15739823E-04
0.78271001E+04	0.15595515E-04
0.79566001E+04	0.15848920E-04
0.79751001E+04	0.15667515E-04
0.79936001E+04	0.15848920E-04
0.81052998E+04	0.15922093E-04
0.81237998E+04	0.16069407E-04
0.81422998E+04	0.15958791E-04
0.81977998E+04	0.16255479E-04
0.83462998E+04	0.15958791E-04
0.83647998E+04	0.15995573E-04
0.83832998E+04	0.16106444E-04
0.84017998E+04	0.16069407E-04
0.84757998E+04	0.16106444E-04
0.85130996E+04	0.16106444E-04
0.85687998E+04	0.15958791E-04
0.86057998E+04	0.15995573E-04
0.87730000E+04	0.16213099E-04
0.88285000E+04	0.16069407E-04
0.88635000E+04	0.16032454E-04
0.88840000E+04	0.16180806E-04
0.89560000E+04	0.15995573E-04
0.89765000E+04	0.16143596E-04
0.90140996E+04	0.16106444E-04

Table B-3

Data for Mustard Hydrolysis at 293 K

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.18709999E+02	0.10023051E-06
0.37209999E+02	0.10839259E-06
0.55709999E+02	0.11534524E-06
0.74209999E+02	0.12531407E-06
0.92709999E+02	0.13273942E-06
0.11121000E+03	0.13995869E-06
0.12971001E+03	0.14487706E-06
0.14821001E+03	0.14927937E-06
0.16672000E+03	0.15275663E-06
0.18522000E+03	0.16143596E-06
0.20372000E+03	0.17377988E-06
0.22222000E+03	0.18706818E-06
0.24122000E+03	0.19906716E-06
0.25972000E+03	0.21134885E-06
0.27822000E+03	0.22335708E-06
0.29672000E+03	0.23067454E-06
0.31522000E+03	0.23988324E-06
0.33372000E+03	0.24831314E-06
0.35222000E+03	0.25644820E-06
0.37072000E+03	0.26791682E-06
0.38923001E+03	0.28575897E-06
0.40773001E+03	0.30549214E-06
0.42623001E+03	0.32508740E-06
0.44473001E+03	0.33962527E-06
0.46323001E+03	0.35399708E-06
0.48239001E+03	0.36982760E-06
0.50089001E+03	0.38194383E-06
0.51939001E+03	0.39264478E-06
0.53789001E+03	0.40644335E-06
0.55639001E+03	0.42657948E-06
0.57489001E+03	0.45081649E-06
0.59339001E+03	0.47973379E-06
0.61189001E+03	0.49545048E-06
0.63039001E+03	0.51522824E-06
0.64889001E+03	0.53579657E-06
0.66739001E+03	0.55080801E-06
0.68589001E+03	0.56885318E-06
0.70439001E+03	0.59156110E-06
0.72339001E+03	0.61944070E-06
0.74188000E+03	0.64863423E-06
0.76039001E+03	0.67608289E-06
0.77889001E+03	0.70957753E-06
0.79739001E+03	0.74130980E-06
0.81588000E+03	0.76207914E-06
0.83438000E+03	0.80723527E-06
0.85289001E+03	0.82413766E-06
0.87138000E+03	0.85113749E-06
0.88988000E+03	0.88920115E-06
0.90839001E+03	0.92682996E-06
0.92689001E+03	0.96605118E-06
0.94538000E+03	0.10115791E-05
0.96388000E+03	0.10568178E-05
0.98304999E+03	0.11015388E-05
0.10016000E+04	0.11455130E-05
0.10201000E+04	0.11885013E-05
0.10386000E+04	0.12274393E-05
0.10571000E+04	0.12852871E-05
0.10756000E+04	0.13365955E-05
0.10941000E+04	0.13963679E-05
0.11126000E+04	0.14621771E-05
0.11311000E+04	0.15205484E-05
0.11496000E+04	0.15812468E-05
0.11680000E+04	0.16634135E-05
0.11865000E+04	0.17298149E-05
0.12050000E+04	0.18071739E-05
0.12242000E+04	0.18836491E-05
0.12427000E+04	0.19815261E-05
0.12612000E+04	0.20606301E-05
0.12797000E+04	0.21478288E-05
0.12982000E+04	0.22542395E-05
0.13167000E+04	0.23550510E-05
0.13352000E+04	0.24717233E-05
0.13537000E+04	0.26121595E-05
0.13722000E+04	0.26915336E-05
0.13907000E+04	0.28444613E-05
0.14092000E+04	0.29553825E-05
0.14277000E+04	0.31260772E-05
0.14462000E+04	0.32734056E-05
0.14652000E+04	0.34276773E-05
0.14837000E+04	0.35892162E-05
0.15022000E+04	0.37583720E-05
0.15207000E+04	0.39084089E-05
0.15392000E+04	0.41114949E-05
0.15577000E+04	0.42854836E-05
0.15762000E+04	0.44565631E-05
0.15947000E+04	0.46558607E-05
0.16132000E+04	0.48305878E-05
0.16317000E+04	0.50350068E-05
0.16502000E+04	0.52601717E-05
0.16687000E+04	0.54200100E-05
0.16872000E+04	0.56234144E-05
0.17064000E+04	0.58479054E-05
0.17249000E+04	0.60953630E-05
0.17434000E+04	0.62805793E-05
0.17619000E+04	0.65313047E-05
0.17804000E+04	0.67608257E-05
0.17989000E+04	0.69342555E-05
0.18174000E+04	0.70957726E-05
0.18359000E+04	0.73282395E-05
0.18544000E+04	0.75509183E-05
0.18729000E+04	0.77983041E-05
0.18914000E+04	0.80352665E-05
0.19099000E+04	0.81658291E-05
0.19284000E+04	0.83945952E-05
0.19475000E+04	0.86496775E-05
0.19660000E+04	0.88307979E-05
0.19845000E+04	0.90157109E-05
0.20030000E+04	0.92257196E-05
0.20215000E+04	0.94188927E-05
0.20400000E+04	0.96382928E-05
0.20585000E+0	0.98401142E-05
0.20770000E+04	0.10092534E-04
0.20955000E+	0.10280164E-04
0.21140000E+04	0.10423179E-04
0.21325000E+04	0.10543862E-04
0.21510000E+04	0.10789467E-04
0.21695000E+04	0.10914401E-04
0.21885000E+04	0.11066239E-04
0.22070000E+04	0.11246051E-04
0.22255000E+04	0.11428784E-04
0.22440000E+04	0.11587778E-04
0.22625000E+04	0.11803206E-04

Table B-3 (continued)

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.22810000E+04	0.12022639E-04
0.22995000E+04	0.12217990E-04
0.23180000E+04	0.12331045E-04
0.23365000E+04	0.12473842E-04
0.23550000E+04	0.12618268E-04
0.23735000E+04	0.12705742E-04
0.23920000E+04	0.12852865E-04
0.24105000E+04	0.12949953E-04
0.24297000E+04	0.13121999E-04
0.24482000E+04	0.13273941E-04
0.24667000E+04	0.13365949E-04
0.24852000E+04	0.13583127E-04
0.25037000E+04	0.13708814E-04
0.25222000E+04	0.13867565E-04
0.25407000E+04	0.14060461E-04
0.25592000E+04	0.14060461E-04
0.25777000E+04	0.14157932E-04
0.25962000E+04	0.14223284E-04
0.26147000E+04	0.14454393E-04
0.26332000E+04	0.14421155E-04
0.26517000E+04	0.14588141E-04
0.26708999E+04	0.14655479E-04
0.26893999E+04	0.14893611E-04
0.27078999E+04	0.14962358E-04
0.27263999E+04	0.15100793E-04
0.27448999E+04	0.15170511E-04
0.27633999E+04	0.15310872E-04
0.27818999E+04	0.15346161E-04
0.28003999E+04	0.15205476E-04
0.28188999E+04	0.15417012E-04
0.28373999E+04	0.15452544E-04
0.28558999E+04	0.15523872E-04
0.28743999E+04	0.15559652E-04
0.28928999E+04	0.15631460E-04
0.29113999E+04	0.15848920E-04
0.29303999E+04	0.15885480E-04
0.29488999E+04	0.16032454E-04
0.29673999E+04	0.16106444E-04
0.29858999E+04	0.16218099E-04
0.30043999E+04	0.16368167E-04
0.30228999E+04	0.16292961E-04
0.30413999E+04	0.16443722E-04
0.30598999E+04	0.16330512E-04
0.30783999E+04	0.16330512E-04
0.30968999E+04	0.16368167E-04
0.31153999E+04	0.16405909E-04
0.31338999E+04	0.16481621E-04
0.31523999E+04	0.16519609E-04
0.31716001E+04	0.16634129E-04
0.31901001E+04	0.16710910E-04
0.32086001E+04	0.16788030E-04
0.32271001E+04	0.16943372E-04
0.32456001E+04	0.17021581E-04
0.32641001E+04	0.17100136E-04
0.32826001E+04	0.17021581E-04
0.33011001E+04	0.17139580E-04
0.33196001E+04	0.16982440E-04
0.33381001E+04	0.17060813E-04
0.33566001E+04	0.17100136E-04
0.33751001E+04	0.17100136E-04
0.33936001E+04	0.17179083E-04
0.34126001E+04	0.17179083E-04
0.34311001E+04	0.17179083E-04
0.34496001E+04	0.17218679E-04
0.34681001E+04	0.17218679E-04
0.34866001E+04	0.17258380E-04
0.35051001E+04	0.17218679E-04
0.35236001E+04	0.17298158E-04
0.35421001E+04	0.17418075E-04
0.35606001E+04	0.17418075E-04
0.35791001E+04	0.17498460E-04
0.35976001E+04	0.17498460E-04
0.36161001E+04	0.17458220E-04
0.36346001E+04	0.17418075E-04
0.36538000E+04	0.17538807E-04
0.36723000E+04	0.17660392E-04
0.36908000E+04	0.17660392E-04
0.37093000E+04	0.17660392E-04
0.37278000E+04	0.17823788E-04
0.37463000E+04	0.17906044E-04
0.37648000E+04	0.18030174E-04
0.37833000E+04	0.18071731E-04
0.38018000E+04	0.18113400E-04
0.38203000E+04	0.18030174E-04
0.38388000E+04	0.18030174E-04
0.38573000E+04	0.17947348E-04
0.38758000E+04	0.17906044E-04
0.38950000E+04	0.17864870E-04
0.39135000E+04	0.17906044E-04
0.39320000E+04	0.17823788E-04
0.39505000E+04	0.17864870E-04
0.39690000E+04	0.17864870E-04
0.39875000E+04	0.17823788E-04
0.40060000E+04	0.17864870E-04
0.40245000E+04	0.18030174E-04
0.40430000E+04	0.17988714E-04
0.40615000E+04	0.17906044E-04
0.40800000E+04	0.17947348E-04
0.40983999E+04	0.17988714E-04
0.41168999E+04	0.18071731E-04
0.41358999E+04	0.18155150E-04
0.41543999E+04	0.18113400E-04
0.41728999E+04	0.18155150E-04
0.41913999E+04	0.18155150E-04
0.42098999E+04	0.18281007E-04
0.42283999E+04	0.18281007E-04
0.42468999E+04	0.18407720E-04
0.42653999E+04	0.18365372E-04
0.42838999E+04	0.18365372E-04
0.43023999E+04	0.18365372E-04
0.43208999E+04	0.18365372E-04
0.43393999E+04	0.18365372E-04
0.43578999E+04	0.18281007E-04
0.43771001E+04	0.18323140E-04
0.43956001E+04	0.18238969E-04
0.44141001E+04	0.18281007E-04
0.44326001E+04	0.18197010E-04
0.44511001E+04	0.13155150E-04
0.44696001E+04	0.18155150E-04
0.44881001E+04	0.18071731E-04
0.45066001E+04	0.18197010E-04
0.45251001E+04	0.18197010E-04

Table B-3 (continued)

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.45436001E+04	0.18155150E-04
0.45621001E+04	0.18155150E-04
0.45806001E+04	0.18238969E-04
0.45991001E+04	0.18323140E-04
0.46182002E+04	0.18238969E-04
0.46367002E+04	0.18323140E-04
0.46552002E+04	0.18281007E-04
0.46737002E+04	0.18365372E-04
0.46922002E+04	0.18407720E-04
0.47107002E+04	0.18535327E-04
0.47292002E+04	0.18578048E-04
0.47477002E+04	0.18620867E-04
0.47662002E+04	0.18578048E-04
0.47847002E+04	0.18578048E-04
0.48032002E+04	0.18492687E-04
0.48217002E+04	0.18535327E-04
0.48402002E+04	0.18578048E-04
0.48587002E+04	0.18450146E-04
0.48777002E+04	0.18535327E-04
0.48962002E+04	0.18450146E-04
0.49147002E+04	0.18407720E-04
0.49332002E+04	0.18323140E-04
0.49517002E+04	0.18281007E-04
0.49702002E+04	0.18281007E-04
0.49887002E+04	0.18323140E-04
0.50072002E+04	0.18323140E-04
0.50257002E+04	0.18365372E-04
0.50442002E+04	0.18365372E-04
0.50627998E+04	0.18281007E-04
0.50812998E+04	0.18407720E-04
0.50997998E+04	0.18450146E-04
0.51188999E+04	0.18535327E-04
0.51373999E+04	0.18535327E-04
0.51558999E+04	0.18535327E-04
0.51743999E+04	0.18620867E-04
0.51928999E+04	0.18620867E-04
0.52113999E+04	0.18620867E-04
0.52298999E+04	0.18706820E-04
0.52483999E+04	0.18793169E-04
0.52668999E+04	0.18663784E-04
0.52853999E+04	0.18706820E-04
0.53040000E+04	0.18749935E-04
0.53225000E+04	0.18706820E-04
0.53410000E+04	0.18578048E-04
0.53601001E+04	0.18663784E-04
0.53786001E+04	0.18663784E-04
0.53971001E+04	0.18492687E-04

Table B-3 (continued)

(a) Cell Two

Time (sec)	$[H^+]$ (M)
0.20170000E+02	0.72945745E-07
0.38669998E+02	0.70957718E-07
0.57169998E+02	0.70145482E-07
0.75680000E+02	0.72610653E-07
0.94180000E+02	0.73620726E-07
0.11268000E+03	0.82413720E-07
0.13117999E+03	0.89949786E-07
0.14967999E+03	0.92257103E-07
0.16819000E+03	0.10046152E-06
0.18669000E+03	0.10568174E-06
0.20519000E+03	0.11220190E-06
0.22389999E+03	0.12022637E-06
0.24269000E+03	0.13001691E-06
0.26119000E+03	0.13677288E-06
0.27969000E+03	0.14421154E-06
0.29819000E+03	0.15346160E-06
0.31669000E+03	0.15848920E-06
0.33519000E+03	0.16180805E-06
0.35369000E+03	0.17060812E-06
0.37219000E+03	0.17579229E-06
0.39069000E+03	0.18879915E-06
0.40919000E+03	0.19952635E-06
0.42769000E+03	0.20511609E-06
0.44619000E+03	0.22029262E-06
0.46512000E+03	0.22698632E-06
0.48385999E+03	0.23988324E-06
0.50235999E+03	0.25003428E-06
0.52085999E+03	0.25703952E-06
0.53934998E+03	0.26977409E-06
0.55784998E+03	0.27542279E-06
0.57634998E+03	0.28707802E-06
0.59484998E+03	0.29922617E-06
0.61334998E+03	0.31622761E-06
0.63184998E+03	0.32809515E-06
0.65034998E+03	0.34355759E-06
0.66884998E+03	0.35809646E-06
0.68734998E+03	0.36043746E-06
0.70615997E+03	0.38194353E-06
0.72484998E+03	0.38547639E-06
0.74334998E+03	0.39354975E-06
0.76184998E+03	0.42072645E-06
0.78034998E+03	0.44360846E-06
0.79885999E+03	0.46773494E-06
0.81734998E+03	0.47533499E-06
0.83584998E+03	0.50234257E-06
0.85434998E+03	0.52119475E-06
0.87284998E+03	0.53703150E-06
0.89134998E+03	0.54954035E-06
0.90984998E+03	0.56623895E-06
0.92834998E+03	0.57676641E-06
0.94684998E+03	0.60394871E-06
0.96569000E+03	0.62661337E-06
0.98451001E+03	0.64268795E-06
0.10030000E+04	0.67608269E-06
0.10215000E+04	0.69502408E-06
0.10400000E+04	0.71285291E-06
0.10585000E+04	0.73451400E-06
0.10770000E+04	0.75162274E-06
0.10955000E+04	0.77268027E-06
0.11140000E+04	0.79799429E-06
0.11325000E+04	0.82224250E-06
0.11510000E+04	0.84139549E-06
0.11695000E+04	0.85901314E-06
0.11880000E+04	0.89536451E-06
0.12069000E+04	0.91201105E-06
0.12257000E+04	0.93110725E-06
0.12442000E+04	0.94623647E-06
0.12627000E+04	0.99311615E-06
0.12812000E+04	0.10092530E-05
0.12997000E+04	0.10399265E-05
0.13182000E+04	0.10739835E-05
0.13367000E+04	0.11066245E-05
0.13552000E+04	0.11323996E-05
0.13737000E+04	0.11614480E-05
0.13922000E+04	0.11830416E-05
0.14107000E+04	0.12246156E-05
0.14292000E+04	0.12502597E-05
0.14479000E+04	0.13001665E-05
0.14667000E+04	0.13335207E-05
0.14852000E+04	0.13899534E-05
0.15037000E+04	0.14092886E-05
0.15222000E+04	0.14421148E-05
0.15407000E+04	0.14927930E-05
0.15592000E+04	0.15275656E-05
0.15777000E+04	0.15595522E-05
0.15962000E+04	0.16032446E-05
0.16147000E+04	0.16405901E-05
0.16332000E+04	0.17060820E-05
0.16517000E+04	0.17619756E-05
0.16702000E+04	0.18071739E-05
0.16890000E+04	0.18365381E-05
0.17078000E+04	0.19054605E-05
0.17263000E+04	0.19815261E-05
0.17448000E+04	0.20558916E-05
0.17633000E+04	0.21183607E-05
0.17818000E+04	0.23227378E-05
0.18003000E+04	0.22335719E-05
0.18188000E+04	0.23067466E-05
0.18373000E+04	0.23823186E-05
0.18558000E+04	0.24490619E-05
0.18743000E+04	0.25234801E-05
0.18928000E+04	0.25822612E-05
0.19113000E+04	0.26302678E-05
0.19302000E+04	0.27289777E-05
0.19490000E+04	0.27989818E-05
0.19675000E+04	0.29040204E-05
0.19860000E+04	0.29512069E-05
0.20045000E+04	0.30199510E-05
0.20230000E+04	0.30690212E-05
0.20415000E+04	0.31695603E-05
0.20600000E+04	0.32734056E-05
0.20785000E+04	0.33728727E-05
0.20970000E+04	0.34119262E-05
0.21155000E+04	0.35399726E-05
0.21340000E+04	0.36475362E-05
0.21525000E+04	0.37068037E-05
0.21713000E+04	0.37844263E-05
0.21900000E+04	0.38635667E-05
0.22085000E+04	0.39902457E-05
0.22270000E+04	0.40550817E-05
0.22455000E+04	0.41399971E-05
0.22640000E+04	0.42268829E-05

Table B-3 (continued)

(a) Cell Two

Time (sec)	$[H^+]$ (M)
0.22825000E+04	0.43451023E-05
0.23010000E+04	0.43853079E-05
0.23195000E+04	0.45289762E-05
0.23380000E+04	0.45919824E-05
0.23565000E+04	0.47206272E-05
0.23750000E+04	0.47533522E-05
0.23935000E+04	0.48305878E-05
0.24123000E+04	0.49888440E-05
0.24312000E+04	0.50234265E-05
0.24497000E+04	0.51286120E-05
0.24682000E+04	0.51522852E-05
0.24867000E+04	0.52480709E-05
0.25052000E+04	0.53703175E-05
0.25237000E+04	0.54200100E-05
0.25422000E+04	0.55975765E-05
0.25607000E+04	0.56493664E-05
0.25792000E+04	0.58210303E-05
0.25977000E+04	0.59292463E-05
0.26162000E+04	0.60255965E-05
0.26347000E+04	0.61801602E-05
0.26536001E+04	0.62230033E-05
0.26723000E+04	0.63679531E-05
0.26908000E+04	0.64120982E-05
0.27093000E+04	0.64416895E-05
0.27278999E+04	0.65614527E-05
0.27463999E+04	0.66221669E-05
0.27648999E+04	0.67297683E-05
0.27833999E+04	0.68076938E-05
0.28018999E+04	0.70631763E-05
0.28203999E+04	0.70307228E-05
0.28388999E+04	0.70957726E-05
0.28573999E+04	0.71121403E-05
0.28758999E+04	0.72777939E-05
0.28943999E+04	0.73113679E-05
0.29132000E+04	0.73451433E-05
0.29318999E+04	0.74301679E-05
0.29503999E+04	0.74473205E-05
0.29688999E+04	0.77268069E-05
0.29873999E+04	0.76207880E-05
0.30058999E+04	0.76913038E-05
0.30243999E+04	0.75857802E-05
0.30428999E+04	0.78162775E-05
0.30613999E+04	0.79067840E-05
0.30798999E+04	0.79799474E-05
0.30983999E+04	0.79250158E-05
0.31168999E+04	0.79799474E-05
0.31353999E+04	0.80537366E-05
0.31543000E+04	0.82035140E-05
0.31731001E+04	0.80909540E-05
0.31916001E+04	0.81546492E-05
0.32101001E+04	0.81096105E-05
0.32286001E+04	0.82413808E-05
0.32471001E+04	0.82035140E-05
0.32656001E+04	0.82794222E-05
0.32841001E+04	0.82985125E-05
0.33026001E+04	0.84527892E-05
0.33211001E+04	0.84722715E-05
0.33396001E+04	0.86496775E-05
0.33581001E+04	0.85901356E-05
0.33766001E+04	0.84917933E-05
0.33953999E+04	0.85703823E-05
0.34141001E+04	0.85703823E-05
0.34326001E+04	0.86496775E-05
0.34511001E+04	0.86396034E-05
0.34696001E+04	0.86696218E-05
0.34881001E+04	0.85901356E-05
0.35066001E+04	0.87297140E-05
0.35251001E+04	0.86496775E-05
0.35436001E+04	0.87498347E-05
0.35621001E+04	0.85703823E-05
0.35806001E+04	0.86396034E-05
0.35991001E+04	0.85901356E-05
0.36176001E+04	0.85901356E-05
0.36363999E+04	0.88920069E-05
0.36553000E+04	0.89330606E-05
0.36738000E+04	0.90364902E-05
0.36922000E+04	0.89536497E-05
0.37107000E+04	0.89125015E-05
0.37292000E+04	0.89330606E-05
0.37477000E+04	0.89330606E-05
0.37662000E+04	0.89949708E-05
0.37847000E+04	0.88307979E-05
0.38032000E+04	0.90157109E-05
0.38217000E+04	0.89536497E-05
0.38403000E+04	0.89949708E-05
0.38588000E+04	0.89330606E-05
0.38777000E+04	0.89536497E-05
0.38963999E+04	0.92469827E-05
0.39148999E+04	0.92044957E-05
0.39333999E+04	0.92044957E-05
0.39518999E+04	0.92469827E-05
0.39703999E+04	0.93540566E-05
0.39888999E+04	0.92257196E-05
0.40073999E+04	0.93325380E-05
0.40253999E+04	0.92896571E-05
0.40443999E+04	0.92044957E-05
0.40628999E+04	0.92469827E-05
0.40813999E+04	0.93325380E-05
0.40998999E+04	0.93110775E-05
0.41187002E+04	0.91833208E-05
0.41373999E+04	0.92896571E-05
0.41558999E+04	0.92469827E-05
0.41743999E+04	0.92044957E-05
0.41928999E+04	0.93972340E-05
0.42113999E+04	0.92257196E-05
0.42298999E+04	0.92257196E-05
0.42483999E+04	0.91622042E-05
0.42668999E+04	0.93110775E-05
0.42853999E+04	0.91411266E-05
0.43038999E+04	0.91833208E-05
0.43223999E+04	0.91411266E-05
0.43408999E+04	0.91622042E-05
0.43597002E+04	0.91201064E-05
0.43785000E+04	0.91622042E-05
0.43970000E+04	0.91833208E-05
0.44155000E+04	0.92682958E-05
0.44340000E+04	0.90782105E-05
0.44525000E+04	0.93110775E-05
0.44710000E+04	0.91411266E-05
0.44895000E+04	0.91201064E-05
0.45080000E+04	0.91833208E-05
0.45265000E+04	0.89949708E-05

Table B-3 (concluded)

(a) Cell Two

Time (sec)	$[H^+]$ (M)
0.45450000E+04	0.90991343E-05
0.45635000E+04	0.91833208E-05
0.45820000E+04	0.91201064E-05
0.46003999E+04	0.90991343E-05
0.46197002E+04	0.92044957E-05
0.46382002E+04	0.91411266E-05
0.46567002E+04	0.90991343E-05
0.46752002E+04	0.91622042E-05
0.46937002E+04	0.91833208E-05
0.47122002E+04	0.93110775E-05
0.47307002E+04	0.92469827E-05
0.47492002E+04	0.92682958E-05
0.47677002E+04	0.91411266E-05
0.47862002E+04	0.92469827E-05
0.48047002E+04	0.93110775E-05
0.48232002E+04	0.92469827E-05
0.48417002E+04	0.93325380E-05
0.48605000E+04	0.94188927E-05
0.48792002E+04	0.94188927E-05
0.48977002E+04	0.94406014E-05
0.49162002E+04	0.95279656E-05
0.49347002E+04	0.94623701E-05
0.49532002E+04	0.94406014E-05
0.49717002E+04	0.94623701E-05
0.49902002E+04	0.94188927E-05
0.50087002E+04	0.94188927E-05
0.50272002E+04	0.94841880E-05
0.50457002E+04	0.93540566E-05
0.50642002E+04	0.93325380E-05
0.50827002E+04	0.95060468E-05
0.51016001E+04	0.94188927E-05
0.51203999E+04	0.93756244E-05
0.51388999E+04	0.92896571E-05
0.51573999E+04	0.93972340E-05
0.51758999E+04	0.92896571E-05
0.51943999E+04	0.93110775E-05
0.52128999E+04	0.93325380E-05
0.52313999E+04	0.93540566E-05
0.52498999E+04	0.93756244E-05
0.52683999E+04	0.92469827E-05
0.52868999E+04	0.94406014E-05
0.53053999E+04	0.93972340E-05
0.53238999E+04	0.94841880E-05
0.53427998E+04	0.93972340E-05
0.53616001E+04	0.94406014E-05
0.53801001E+04	0.93972340E-05
0.53986001E+04	0.93756244E-05

Table B-4

Data for Mustard Hydrolysis at 298 K

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.18700001E+02	0.97949012E-07
0.37200001E+02	0.17139569E-06
0.55700001E+02	0.29308950E-06
0.74199997E+02	0.48640630E-06
0.92699997E+02	0.79432851E-06
0.11120000E+03	0.12971786E-05
0.12970000E+03	0.21086275E-05
0.14620000E+03	0.33806455E-05
0.16670000E+03	0.49431051E-05
0.18520000E+03	0.67297683E-05
0.20369000E+03	0.85506063E-05
0.22219000E+03	0.10543662E-04
0.24135001E+03	0.12615263E-04
0.25985001E+03	0.14655479E-04
0.27635001E+03	0.16572469E-04
0.29635001E+03	0.18653764E-04
0.31535001E+03	0.20556955E-04
0.33365001E+03	0.22433508E-04
0.35235001E+03	0.24210271E-04
0.37085001E+03	0.25941748E-04
0.38934000E+03	0.27797107E-04
0.40785001E+03	0.29308932E-04
0.42634000E+03	0.31332832E-04
0.44484000E+03	0.32960965E-04
0.46334000E+03	0.34914061E-04
0.48267001E+03	0.36982753E-04
0.50117001E+03	0.38636688E-04
0.51966998E+03	0.40738013E-04
0.53816998E+03	0.41782994E-04
0.55666998E+03	0.43251399E-04
0.57516998E+03	0.44463090E-04
0.59366998E+03	0.45708817E-04
0.61216998E+03	0.47097699E-04
0.63066998E+03	0.48083952E-04
0.64916998E+03	0.49559244E-04
0.66766998E+03	0.50933260E-04
0.68616998E+03	0.52420736E-04
0.70466998E+03	0.53951040E-04
0.72365997E+03	0.55718549E-04
0.74215997E+03	0.57147849E-04
0.76066998E+03	0.58344496E-04
0.77916998E+03	0.59566204E-04
0.79766998E+03	0.60534076E-04
0.81616998E+03	0.61094150E-04
0.83466998E+03	0.61944076E-04
0.85316998E+03	0.62661540E-04
0.87166998E+03	0.63241219E-04
0.89016998E+03	0.63826337E-04
0.90866998E+03	0.64714200E-04
0.92716998E+03	0.65313005E-04
0.94566996E+03	0.66374334E-04
0.96416998E+03	0.67142901E-04
0.98333002E+03	0.68865193E-04
0.10014000E+04	0.69823228E-04
0.10203000E+04	0.70957759E-04
0.10388000E+04	0.71614340E-04
0.10573000E+04	0.71944936E-04
0.10758000E+04	0.71944836E-04
0.10943000E+04	0.72276948E-04
0.11128000E+04	0.72945717E-04
0.11313000E+04	0.73282426E-04
0.11498000E+04	0.73960524E-04
0.11683000E+04	0.75335513E-04
0.11868000E+04	0.76207922E-04
0.12053000E+04	0.76913073E-04
0.12245000E+04	0.77268029E-04
0.12430000E+04	0.77624696E-04
0.12615000E+04	0.77090350E-04
0.12800000E+04	0.77624696E-04
0.12985000E+04	0.77624696E-04
0.13170000E+04	0.78162811E-04
0.13355000E+04	0.79250123E-04
0.13540000E+04	0.80352627E-04
0.13725000E+04	0.81096070E-04
0.13910000E+04	0.81652254E-04
0.14095000E+04	0.81282932E-04
0.14280000E+04	0.81096070E-04
0.14465000E+04	0.81096070E-04
0.14657000E+04	0.81282932E-04
0.14842000E+04	0.81646461E-04
0.15027000E+04	0.82063714E-04
0.15212000E+04	0.83752879E-04
0.15397000E+04	0.84333465E-04
0.15582000E+04	0.84139559E-04
0.15767000E+04	0.83752879E-04
0.15952000E+04	0.83368141E-04
0.16137000E+04	0.83752879E-04
0.16322000E+04	0.84139559E-04
0.16507000E+04	0.84527856E-04
0.16692000E+04	0.84918029E-04
0.16877000E+04	0.86099390E-04
0.17070000E+04	0.86696178E-04
0.17255000E+04	0.86297554E-04
0.17440000E+04	0.85901323E-04
0.17625000E+04	0.85506712E-04
0.17810000E+04	0.85310086E-04
0.17995000E+04	0.85703798E-04
0.18180000E+04	0.86696178E-04
0.18365000E+04	0.87297100E-04
0.18550000E+04	0.87700057E-04
0.18735000E+04	0.87700057E-04
0.18920000E+04	0.87096356E-04
0.19105000E+04	0.86696178E-04
0.19290000E+04	0.86896079E-04
0.19482000E+04	0.87902190E-04
0.19667000E+04	0.86715562E-04
0.19852000E+04	0.88920118E-04
0.20037000E+04	0.88303021E-04
0.20222000E+04	0.87495379E-04
0.20407000E+04	0.87496354E-04
0.20592000E+04	0.87902190E-04
0.20777000E+04	0.88308021E-04
0.20962000E+04	0.89536457E-04
0.21147000E+04	0.89949746E-04
0.21332000E+04	0.89125069E-04
0.21517000E+04	0.87902190E-04
0.21702000E+04	0.87902190E-04
0.21893999E+04	0.86715562E-04
0.22078999E+04	0.89536457E-04
0.22263999E+04	0.89949746E-04
0.22446999E+04	0.89742965E-04
0.22633999E+04	0.89125062E-04

Table B-4 (continued)

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.22818999E+04	0.88308021E-04
0.23003999E+04	0.88511559E-04
0.23188999E+04	0.88920119E-04
0.23373999E+04	0.89536457E-04
0.23558999E+04	0.90573223E-04
0.23743999E+04	0.90782065E-04
0.23928999E+04	0.90157067E-04
0.24113999E+04	0.89536457E-04
0.24307000E+04	0.88920119E-04
0.24492000E+04	0.89330570E-04
0.24677000E+04	0.90157067E-04
0.24862000E+04	0.90782065E-04
0.25047000E+04	0.90991307E-04
0.25232000E+04	0.90573223E-04
0.25417000E+04	0.89742905E-04
0.25602000E+04	0.89330570E-04
0.25787000E+04	0.88920119E-04
0.25972000E+04	0.89330570E-04
0.26157000E+04	0.89949746E-04
0.26342000E+04	0.90573223E-04
0.26527000E+04	0.90991307E-04
0.26713999E+04	0.90782065E-04
0.26903999E+04	0.90364862E-04
0.27088999E+04	0.89949746E-04
0.27273999E+04	0.89536457E-04
0.27458999E+04	0.89330570E-04
0.27643999E+04	0.89742905E-04
0.27828999E+04	0.89742905E-04
0.28013999E+04	0.90364862E-04
0.28198999E+04	0.91201109E-04
0.28383999E+04	0.91201109E-04
0.28568999E+04	0.91411312E-04
0.28753999E+04	0.90991307E-04
0.28938999E+04	0.90364862E-04
0.29123999E+04	0.89949746E-04
0.29313999E+04	0.89742905E-04
0.29498999E+04	0.89742905E-04
0.29683999E+04	0.90364862E-04
0.29868999E+04	0.90991307E-04
0.30053999E+04	0.91411312E-04
0.30238999E+04	0.91833172E-04
0.30423999E+04	0.92045004E-04
0.30608999E+04	0.91833172E-04
0.30793999E+04	0.91411312E-04
0.30978999E+04	0.90782065E-04
0.31163999E+04	0.90573223E-04
0.31348999E+04	0.90364862E-04
0.31533999E+04	0.89949746E-04
0.31726001E+04	0.90364862E-04
0.31911001E+04	0.90991307E-04
0.32096001E+04	0.91201109E-04
0.32281001E+04	0.91622001E-04
0.32466001E+04	0.92045004E-04
0.32651001E+04	0.92257156E-04
0.32836001E+04	0.91833172E-04
0.33021001E+04	0.91411312E-04
0.33206001E+04	0.90991307E-04
0.33391001E+04	0.90573223E-04
0.33576001E+04	0.90364862E-04
0.33761001E+04	0.90782065E-04
0.33946001E+04	0.90991307E-04
0.34135000E+04	0.91833172E-04
0.34322000E+04	0.92045004E-04
0.34507000E+04	0.92045004E-04
0.34692000E+04	0.92257156E-04
0.34877000E+04	0.91833172E-04
0.35062000E+04	0.91622001E-04
0.35247000E+04	0.90991307E-04
0.35432000E+04	0.90573223E-04
0.35617000E+04	0.90573223E-04
0.35802000E+04	0.90364862E-04
0.35987000E+04	0.90782065E-04
0.36172000E+04	0.91201109E-04
0.36357000E+04	0.91411312E-04
0.36547000E+04	0.92257156E-04
0.36732000E+04	0.92257156E-04
0.36917000E+04	0.91833172E-04
0.37102000E+04	0.91411312E-04
0.37287000E+04	0.90991307E-04
0.37472000E+04	0.90991307E-04
0.37657000E+04	0.90573223E-04
0.37842000E+04	0.90991307E-04
0.38027000E+04	0.91201109E-04
0.38212000E+04	0.91833172E-04
0.38397000E+04	0.92469789E-04
0.38582000E+04	0.92683033E-04
0.38767000E+04	0.91833172E-04
0.38953999E+04	0.90782065E-04
0.39143999E+04	0.90573223E-04
0.39328999E+04	0.90991307E-04
0.39513999E+04	0.91411312E-04
0.39698999E+04	0.92469789E-04
0.39883999E+04	0.92469789E-04
0.40068999E+04	0.91833172E-04
0.40253999E+04	0.90991307E-04
0.40438999E+04	0.90782065E-04
0.40623999E+04	0.90782065E-04
0.40808999E+04	0.90991307E-04
0.40993999E+04	0.91833172E-04
0.41173999E+04	0.92257156E-04
0.41370000E+04	0.92257156E-04
0.41555000E+04	0.91201109E-04
0.41740000E+04	0.90573223E-04
0.41925000E+04	0.90573223E-04
0.42110000E+04	0.90991307E-04
0.42295000E+04	0.91411312E-04
0.42480000E+04	0.92257156E-04
0.42665000E+04	0.92469789E-04
0.42850000E+04	0.92045004E-04
0.43035000E+04	0.91411312E-04
0.43220000E+04	0.90991307E-04
0.43405000E+04	0.90573223E-04
0.43590000E+04	0.90782065E-04
0.43775002E+04	0.92045004E-04
0.43960002E+04	0.92257156E-04
0.44152002E+04	0.92045004E-04
0.44337002E+04	0.91411312E-04
0.44522002E+04	0.90782065E-04
0.44707002E+04	0.90573223E-04
0.44892002E+04	0.90991307E-04
0.45077002E+04	0.91622001E-04
0.45262002E+04	0.92469789E-04

Table B-4 (continued)

(a) Cell One

Time (sec)	[H^+] (M)
0.45447002E+04	0.92257156E-04
0.45632002E+04	0.91333172E-04
0.45517002E+04	0.90991307E-04
0.46002002E+04	0.90782065E-04
0.46192993E+04	0.91201109E-04
0.46377993E+04	0.91333172E-04
0.46562993E+04	0.92257156E-04
0.46747996E+04	0.91522001E-04
0.46932996E+04	0.90991307E-04
0.47117996E+04	0.90573223E-04
0.47302993E+04	0.91201109E-04
0.47487996E+04	0.92045004E-04
0.47672993E+04	0.92469789E-04
0.47857993E+04	0.91622001E-04
0.48042995E+04	0.90991307E-04
0.48227996E+04	0.90991307E-04
0.48412996E+04	0.91201109E-04
0.48597996E+04	0.92045004E-04
0.48783999E+04	0.92045004E-04
0.48973999E+04	0.91201109E-04
0.49158999E+04	0.90782065E-04
0.49343999E+04	0.90782065E-04
0.49523999E+04	0.91201109E-04
0.49713999E+04	0.92045004E-04
0.49898999E+04	0.92257156E-04
0.50083999E+04	0.91622001E-04
0.50268999E+04	0.90573223E-04
0.50453999E+04	0.90573223E-04
0.50638999E+04	0.90782065E-04
0.50823999E+04	0.91411312E-04
0.51003999E+04	0.92257156E-04
0.51202002E+04	0.92045004E-04
0.51387002E+04	0.90991307E-04
0.51572002E+04	0.90991307E-04
0.51757002E+04	0.90782065E-04
0.51942002E+04	0.90991307E-04
0.52127002E+04	0.92257156E-04
0.52312002E+04	0.92257156E-04
0.52497002E+04	0.91411312E-04
0.52682002E+04	0.90991307E-04
0.52867002E+04	0.90782065E-04
0.53052002E+04	0.91622001E-04
0.53237002E+04	0.92257156E-04
0.53422002E+04	0.92469789E-04
0.53615002E+04	0.91201109E-04
0.53800000E+04	0.90782065E-04
0.53985000E+04	0.91411312E-04

Table B-4 (continued)

(b) Cell Two

Time (sec)	[H^+] (M)	Time (sec)	[H^+] (M)
0.61700001E+01	0.40644355E-07	0.11380000E+04	0.65162829E-04
0.24670000E+02	0.83176303E-07	0.11570000E+04	0.64863430E-04
0.43169998E+02	0.16330512E-06	0.11750000E+04	0.65765729E-04
0.61660000E+02	0.25351270E-06	0.11940000E+04	0.66834335E-04
0.80160004E+02	0.34753606E-06	0.12120000E+04	0.67920300E-04
0.98870003E+02	0.48977870E-06	0.12310000E+04	0.68391149E-04
0.11780000E+03	0.71285291E-06	0.12490000E+04	0.68706831E-04
0.13630000E+03	0.10209384E-05	0.12680000E+04	0.69342590E-04
0.15480000E+03	0.14962366E-05	0.12860000E+04	0.67920300E-04
0.17330000E+03	0.22130937E-05	0.13050000E+04	0.70469305E-04
0.19180000E+03	0.32508724E-05	0.13230000E+04	0.68706831E-04
0.21030000E+03	0.45603683E-05	0.13420000E+04	0.71944836E-04
0.22880000E+03	0.59841127E-05	0.13610000E+04	0.70957758E-04
0.24730000E+03	0.75857802E-05	0.13790000E+04	0.71614340E-04
0.26579999E+03	0.93110775E-05	0.13980000E+04	0.73960524E-04
0.28429999E+03	0.11194368E-04	0.14160000E+04	0.75162279E-04
0.30279999E+03	0.12823298E-04	0.14350000E+04	0.74816933E-04
0.32129999E+03	0.14825179E-04	0.14530000E+04	0.74816933E-04
0.34020001E+03	0.16368167E-04	0.14720000E+04	0.75509153E-04
0.35910001E+03	0.18663784E-04	0.14900000E+04	0.75509153E-04
0.37760001E+03	0.19860941E-04	0.15090000E+04	0.76032607E-04
0.39610001E+03	0.23173932E-04	0.15270000E+04	0.76559612E-04
0.41460001E+03	0.24154599E-04	0.15460000E+04	0.77624696E-04
0.43310001E+03	0.25176763E-04	0.15650000E+04	0.77983001E-04
0.45160001E+03	0.27227010E-04	0.15840000E+04	0.77624696E-04
0.47010001E+03	0.28054315E-04	0.16020000E+04	0.77803605E-04
0.48860001E+03	0.30060768E-04	0.16210000E+04	0.78342964E-04
0.50710001E+03	0.31695679E-04	0.16390000E+04	0.77446195E-04
0.52559998E+03	0.33036966E-04	0.16580000E+04	0.78885991E-04
0.54409998E+03	0.33728713E-04	0.16760000E+04	0.79799436E-04
0.56259998E+03	0.35399709E-04	0.16950000E+04	0.80352627E-04
0.58150000E+03	0.36559486E-04	0.17130000E+04	0.81096070E-04
0.60009998E+03	0.38994196E-04	0.17320000E+04	0.81846461E-04
0.61859998E+03	0.39627801E-04	0.17500000E+04	0.80537829E-04
0.63709998E+03	0.41975902E-04	0.17690000E+04	0.79432852E-04
0.65559998E+03	0.41975902E-04	0.17870000E+04	0.79799436E-04
0.67409998E+03	0.43052631E-04	0.18060000E+04	0.80909587E-04
0.69259998E+03	0.43954176E-04	0.18250000E+04	0.81846461E-04
0.71109998E+03	0.45185599E-04	0.18430000E+04	0.83176354E-04
0.72959998E+03	0.46665937E-04	0.18620000E+04	0.82413768E-04
0.74809998E+03	0.47624197E-04	0.18800000E+04	0.81846461E-04
0.76659998E+03	0.48977876E-04	0.18990000E+04	0.82413768E-04
0.78509998E+03	0.49317361E-04	0.19170000E+04	0.82224258E-04
0.80359998E+03	0.51286144E-04	0.19360000E+04	0.83176354E-04
0.82209998E+03	0.51641629E-04	0.19540000E+04	0.82985091E-04
0.84100000E+03	0.53088424E-04	0.19730000E+04	0.82794264E-04
0.85979999E+03	0.54575754E-04	0.19910000E+04	0.83560291E-04
0.87829999E+03	0.55847020E-04	0.20100000E+04	0.82794264E-04
0.89679999E+03	0.56885325E-04	0.20280000E+04	0.82413768E-04
0.91529999E+03	0.56754459E-04	0.20470000E+04	0.83560291E-04
0.93379999E+03	0.57411635E-04	0.20660000E+04	0.81470396E-04
0.95229999E+03	0.59020087E-04	0.20840000E+04	0.82794264E-04
0.97079999E+03	0.58613812E-04	0.21030000E+04	0.82603714E-04
0.98929999E+03	0.59429232E-04	0.21210000E+04	0.81658254E-04
0.10080000E+04	0.59861157E-04	0.21400000E+04	0.83560291E-04
0.10260000E+04	0.61801635E-04	0.21580000E+04	0.82985091E-04
0.10450000E+04	0.61944076E-04	0.21770000E+04	0.83560291E-04
0.10630000E+04	0.63095729E-04	0.21950000E+04	0.83176354E-04
0.10820000E+04	0.62230065E-04	0.22140000E+04	0.82985091E-04
0.11010000E+04	0.64416927E-04	0.22320000E+04	0.84333486E-04
0.11200000E+04	0.64268803E-04	0.22510000E+04	0.83176354E-04

Table B-4 (continued)

(b) Cell Two

Time (sec)	$[H^+]$ (M)	Time (sec)	$[H^+]$ (M)
0.22690000E+04	0.82985091E-04	0.34010000E+04	0.85506712E-04
0.22880000E+04	0.82985091E-04	0.34200000E+04	0.86099390E-04
0.23070000E+04	0.82794264E-04	0.34380000E+04	0.85703788E-04
0.23260000E+04	0.84139559E-04	0.34570000E+04	0.86099390E-04
0.23440000E+04	0.84527856E-04	0.34750000E+04	0.87096356E-04
0.23630000E+04	0.85113752E-04	0.34940000E+04	0.86496737E-04
0.23810000E+04	0.84139559E-04	0.35130000E+04	0.87902190E-04
0.24000000E+04	0.84333486E-04	0.35310000E+04	0.87498389E-04
0.24180000E+04	0.83752879E-04	0.35500000E+04	0.87297100E-04
0.24370000E+04	0.83560291E-04	0.35680000E+04	0.87096356E-04
0.24550000E+04	0.84333486E-04	0.35870000E+04	0.87297100E-04
0.24740000E+04	0.85506712E-04	0.36050000E+04	0.86696178E-04
0.24920000E+04	0.85113752E-04	0.36240000E+04	0.86696178E-04
0.25110000E+04	0.86496737E-04	0.36420000E+04	0.87297100E-04
0.25300000E+04	0.86496737E-04	0.36610000E+04	0.87498389E-04
0.25480000E+04	0.85703788E-04	0.36790000E+04	0.87498389E-04
0.25670000E+04	0.84918029E-04	0.36980000E+04	0.87902190E-04
0.25850000E+04	0.84918029E-04	0.37160000E+04	0.88920118E-04
0.26040000E+04	0.84918029E-04	0.37350000E+04	0.87902190E-04
0.26220000E+04	0.85113752E-04	0.37540000E+04	0.87700057E-04
0.26410000E+04	0.85310086E-04	0.37720000E+04	0.86297834E-04
0.26590000E+04	0.85310086E-04	0.37910000E+04	0.86496737E-04
0.26780000E+04	0.85506712E-04	0.38090000E+04	0.88104869E-04
0.26960000E+04	0.86099390E-04	0.38280000E+04	0.87700057E-04
0.27150000E+04	0.87096356E-04	0.38460000E+04	0.88104869E-04
0.27330000E+04	0.86696178E-04	0.38650000E+04	0.87700057E-04
0.27520000E+04	0.85113752E-04	0.38830000E+04	0.88308021E-04
0.27700000E+04	0.84722757E-04	0.39020000E+04	0.87297100E-04
0.27890000E+04	0.85506712E-04	0.39200000E+04	0.87096356E-04
0.28080000E+04	0.85310086E-04	0.39390000E+04	0.88511559E-04
0.28260000E+04	0.86297834E-04	0.39570000E+04	0.88511559E-04
0.28450000E+04	0.85901323E-04	0.39760000E+04	0.88715562E-04
0.28630000E+04	0.86696178E-04	0.39950000E+04	0.88920118E-04
0.28820000E+04	0.86896078E-04	0.40140000E+04	0.87096356E-04
0.29000000E+04	0.86896078E-04	0.40320000E+04	0.86496737E-04
0.29190000E+04	0.86496737E-04	0.40510000E+04	0.87096356E-04
0.29370000E+04	0.86496737E-04	0.40690000E+04	0.87096356E-04
0.29560000E+04	0.85703788E-04	0.40880000E+04	0.88104869E-04
0.29740000E+04	0.85703788E-04	0.41060000E+04	0.89125060E-04
0.29930000E+04	0.85113752E-04	0.41250000E+04	0.87902190E-04
0.30110000E+04	0.84918029E-04	0.41430000E+04	0.88308021E-04
0.30300000E+04	0.85310086E-04	0.41620000E+04	0.85310086E-04
0.30490000E+04	0.85310086E-04	0.41800000E+04	0.86297834E-04
0.30680000E+04	0.85310086E-04	0.41990000E+04	0.86297834E-04
0.30860000E+04	0.86099390E-04	0.42170000E+04	0.86496737E-04
0.31050000E+04	0.86099390E-04	0.42360000E+04	0.86099390E-04
0.31230000E+04	0.85703788E-04	0.42550000E+04	0.87096356E-04
0.31420000E+04	0.85506712E-04	0.42730000E+04	0.88308021E-04
0.31600000E+04	0.86696178E-04	0.42920000E+04	0.86099390E-04
0.31790000E+04	0.86099390E-04	0.43100000E+04	0.86099390E-04
0.31970000E+04	0.85703788E-04	0.43290000E+04	0.85901323E-04
0.32160000E+04	0.85310086E-04	0.43470000E+04	0.86297834E-04
0.32340000E+04	0.85310086E-04	0.43660000E+04	0.86896078E-04
0.32530000E+04	0.84527856E-04	0.43840000E+04	0.87096356E-04
0.32710000E+04	0.84918029E-04	0.44030000E+04	0.86896078E-04
0.32900000E+04	0.84333486E-04	0.44210000E+04	0.86099390E-04
0.33090000E+04	0.84333486E-04	0.44400000E+04	0.86297834E-04
0.33270000E+04	0.85901323E-04	0.44580000E+04	0.86496737E-04
0.33460000E+04	0.84722757E-04	0.44770000E+04	0.86099390E-04
0.33640000E+04	0.86496737E-04	0.44960000E+04	0.86297834E-04
0.33830000E+04	0.86099390E-04	0.45140000E+04	0.87096356E-04

Table B-4 (concluded)

(b) Cell Two

Time (sec)	$[H^+]$ (M)
0.45330000E+04	0.85901323E-04
0.45510000E+04	0.86896078E-04
0.45700000E+04	0.86896078E-04
0.45880000E+04	0.86696178E-04
0.46070000E+04	0.86896078E-04
0.46250000E+04	0.87902190E-04
0.46440000E+04	0.87700057E-04
0.46620000E+04	0.86896078E-04
0.46810000E+04	0.86297834E-04
0.46990000E+04	0.87297100E-04
0.47120000E+04	0.88104869E-04
0.47370000E+04	0.86099390E-04
0.47550000E+04	0.87498389E-04
0.47740000E+04	0.87096356E-04
0.47920000E+04	0.86896078E-04
0.48110000E+04	0.87700057E-04
0.48290000E+04	0.88511559E-04
0.48480000E+04	0.88308021E-04
0.48660000E+04	0.87096356E-04
0.48850000E+04	0.87297100E-04
0.49030000E+04	0.88308021E-04
0.49220000E+04	0.87902190E-04
0.49400000E+04	0.88308021E-04
0.49590000E+04	0.89125060E-04
0.49780000E+04	0.88920118E-04
0.49970000E+04	0.86696178E-04
0.50150000E+04	0.87096356E-04
0.50340000E+04	0.87094356E-04
0.50520000E+04	0.88715562E-04
0.50710000E+04	0.89125060E-04
0.50890000E+04	0.88715562E-04
0.51080000E+04	0.88715562E-04
0.51260000E+04	0.87498389E-04
0.51450000E+04	0.87498389E-04
0.51630000E+04	0.87700057E-04
0.51820000E+04	0.88920118E-04
0.52000000E+04	0.88715562E-04

Table B-5

Data for Mustard Hydrolysis at 303 K

(a) Cell One

Time (sec)	$[H^+]$ (M)	Time (sec)	$[H^+]$ (M)
0.18700001E+02	0.14757060E-06	0.11499000E+04	0.55590394E-05
0.37209999E+02	0.17179053E-06	0.11684000E+04	0.56363751E-05
0.55709999E+02	0.19906716E-06	0.11869000E+04	0.56104777E-05
0.74209999E+02	0.23067454E-06	0.12054000E+04	0.56493664E-05
0.92709999E+02	0.26853431E-06	0.12245000E+04	0.56363751E-05
0.11122000E+03	0.30690225E-06	0.12430000E+04	0.56493664E-05
0.12972000E+03	0.35156029E-06	0.12615000E+04	0.56754424E-05
0.14822000E+03	0.40086695E-06	0.12800000E+04	0.57016405E-05
0.16672000E+03	0.44977950E-06	0.12985000E+04	0.57147872E-05
0.18522000E+03	0.51168212E-06	0.13170000E+04	0.56885297E-05
0.20372000E+03	0.57676541E-06	0.13355000E+04	0.57809602E-05
0.22221001E+03	0.65012983E-06	0.13540000E+04	0.57411637E-05
0.24121001E+03	0.71944934E-06	0.13725000E+04	0.57544039E-05
0.25970999E+03	0.79933351E-06	0.13910000E+04	0.57809602E-05
0.27820999E+03	0.89536451E-06	0.14095000E+04	0.58076448E-05
0.29670001E+03	0.99770034E-06	0.14280000E+04	0.58613837E-05
0.31520001E+03	0.10964776E-05	0.14465000E+04	0.58479054E-05
0.33370999E+03	0.12246156E-05	0.14657000E+04	0.58344467E-05
0.35220999E+03	0.13365955E-05	0.14842000E+04	0.58884339E-05
0.37070001E+03	0.14757069E-05	0.15027000E+04	0.58479054E-05
0.38920001E+03	0.15885472E-05	0.15212000E+04	0.58613837E-05
0.40770001E+03	0.17218687E-05	0.15397000E+04	0.58479054E-05
0.42620001E+03	0.18749926E-05	0.15582000E+04	0.58479054E-05
0.44470001E+03	0.20137231E-05	0.15767000E+04	0.58344467E-05
0.46320001E+03	0.21727012E-05	0.15952000E+04	0.58613837E-05
0.48235999E+03	0.23334571E-05	0.16137000E+04	0.58613837E-05
0.50085999E+03	0.25003442E-05	0.16322000E+04	0.58344467E-05
0.51935999E+03	0.26668595E-05	0.16507000E+04	0.57809602E-05
0.53785999E+03	0.27925428E-05	0.16692000E+04	0.58344467E-05
0.55635999E+03	0.29376497E-05	0.16877000E+04	0.58210303E-05
0.57485999E+03	0.30690212E-05	0.17070000E+04	0.58344467E-05
0.59335999E+03	0.32210676E-05	0.17255000E+04	0.58344467E-05
0.61185999E+03	0.33573754E-05	0.17440000E+04	0.58884339E-05
0.63035999E+03	0.34914044E-05	0.17625000E+04	0.58613837E-05
0.64885999E+03	0.36307804E-05	0.17810000E+04	0.58479054E-05
0.66735999E+03	0.37411032E-05	0.17995000E+04	0.58613837E-05
0.68585999E+03	0.39084069E-05	0.18180000E+04	0.58344467E-05
0.70435999E+03	0.40271716E-05	0.18365000E+04	0.58884339E-05
0.72369000E+03	0.41495391E-05	0.18550000E+04	0.59020113E-05
0.74219000E+03	0.42169636E-05	0.18735000E+04	0.58884339E-05
0.76069000E+03	0.43151917E-05	0.18920000E+04	0.58748933E-05
0.77919000E+03	0.43954155E-05	0.19105000E+04	0.58884339E-05
0.79769000E+03	0.45051629E-05	0.19290000E+04	0.58884339E-05
0.81619000E+03	0.45708794E-05	0.19481000E+04	0.58884339E-05
0.83469000E+03	0.46989376E-05	0.19666000E+04	0.58748933E-05
0.85319000E+03	0.47973356E-05	0.19851000E+04	0.58344467E-05
0.87169000E+03	0.48640704E-05	0.20036000E+04	0.58479054E-05
0.89019000E+03	0.49545029E-05	0.20221000E+04	0.58884339E-05
0.90869000E+03	0.50118674E-05	0.20406000E+04	0.58748933E-05
0.92719000E+03	0.50582476E-05	0.20591001E+04	0.58613837E-05
0.94569000E+03	0.51168186E-05	0.20776001E+04	0.58613837E-05
0.96419000E+03	0.51641605E-05	0.20961001E+04	0.58344467E-05
0.98335999E+03	0.51760676E-05	0.21146001E+04	0.58613837E-05
0.10019000E+04	0.52360028E-05	0.21331001E+04	0.58344467E-05
0.10204000E+04	0.52844525E-05	0.21516001E+04	0.58613837E-05
0.10389000E+04	0.53333501E-05	0.21701001E+04	0.58210303E-05
0.10574000E+04	0.53703175E-05	0.21891001E+04	0.58210303E-05
0.10759000E+04	0.54450279E-05	0.22076001E+04	0.58479054E-05
0.10944000E+04	0.54954066E-05	0.22261001E+04	0.58479054E-05
0.11129000E+04	0.55335026E-05	0.22446001E+04	0.58344467E-05
0.11314000E+04	0.55590394E-05	0.22631001E+04	0.58344467E-05

Table B-5 (continued)

(a) Cell One

Time (sec)	$[H^+]$ (M)	Time (sec)	$[H^+]$ (M)
0.22816001E+04	0.57942843E-05	0.34135000E+04	0.55335026E-05
0.23001001E+04	0.58076448E-05	0.34320000E+04	0.55207729E-05
0.23186001E+04	0.57942843E-05	0.34505000E+04	0.55080777E-05
0.23371001E+04	0.57809602E-05	0.34690000E+04	0.54701568E-05
0.23556001E+04	0.57942843E-05	0.34875000E+04	0.55207729E-05
0.23741001E+04	0.57676671E-05	0.35060000E+04	0.54954066E-05
0.23926001E+04	0.58076448E-05	0.35245000E+04	0.54701568E-05
0.24111001E+04	0.58076448E-05	0.35430000E+04	0.54954066E-05
0.24303000E+04	0.57544039E-05	0.35615000E+04	0.54954066E-05
0.24488000E+04	0.57942843E-05	0.35800000E+04	0.54954066E-05
0.24673000E+04	0.57809602E-05	0.35985000E+04	0.54954066E-05
0.24858000E+04	0.57809602E-05	0.36170000E+04	0.54827642E-05
0.25043000E+04	0.57942843E-05	0.36355000E+04	0.54954066E-05
0.25228000E+04	0.57544039E-05	0.36547000E+04	0.54954066E-05
0.25413000E+04	0.57411607E-05	0.36732000E+04	0.54701568E-05
0.25598000E+04	0.57544039E-05	0.36917000E+04	0.54450279E-05
0.25783000E+04	0.57544039E-05	0.37102000E+04	0.54575780E-05
0.25968000E+04	0.57279590E-05	0.37287000E+04	0.54701568E-05
0.26153000E+04	0.57279590E-05	0.37472000E+04	0.54325019E-05
0.26338000E+04	0.57147872E-05	0.37657000E+04	0.54325019E-05
0.26523000E+04	0.56885297E-05	0.37841001E+04	0.54200100E-05
0.26716001E+04	0.56885297E-05	0.38026001E+04	0.54325019E-05
0.26901001E+04	0.56754434E-05	0.38211001E+04	0.54200100E-05
0.27086001E+04	0.56754484E-05	0.38396001E+04	0.54450279E-05
0.27271001E+04	0.56623871E-05	0.38581001E+04	0.54325019E-05
0.27456001E+04	0.56754484E-05	0.38766001E+04	0.54325019E-05
0.27641001E+04	0.56623871E-05	0.38958000E+04	0.54200100E-05
0.27826001E+04	0.56363751E-05	0.39143000E+04	0.54075413E-05
0.28011001E+04	0.56493664E-05	0.39328000E+04	0.54075413E-05
0.28196001E+04	0.56234144E-05	0.39513000E+04	0.53951012E-05
0.28381001E+04	0.56623871E-05	0.39698000E+04	0.54075413E-05
0.28566001E+04	0.56623871E-05	0.39883000E+04	0.53826952E-05
0.28751001E+04	0.56104777E-05	0.40068000E+04	0.54200100E-05
0.28936001E+04	0.56363751E-05	0.40253000E+04	0.54200100E-05
0.29121001E+04	0.56754484E-05	0.40438000E+04	0.54325019E-05
0.29311001E+04	0.56363751E-05	0.40623000E+04	0.53826952E-05
0.29496001E+04	0.56104777E-05	0.40808000E+04	0.53951012E-05
0.29681001E+04	0.56104777E-05	0.40992998E+04	0.53579683E-05
0.29866001E+04	0.56104777E-05	0.41177998E+04	0.53579683E-05
0.30051001E+04	0.56104777E-05	0.41371001E+04	0.53579683E-05
0.30236001E+04	0.56104777E-05	0.41556001E+04	0.53456424E-05
0.30421001E+04	0.55847045E-05	0.41741001E+04	0.53579683E-05
0.30606001E+04	0.56104777E-05	0.41926001E+04	0.53826952E-05
0.30791001E+04	0.56104777E-05	0.42111001E+04	0.53703175E-05
0.30976001E+04	0.55975765E-05	0.42296001E+04	0.53703175E-05
0.31161001E+04	0.55847045E-05	0.42481001E+04	0.53210511E-05
0.31346001E+04	0.56104777E-05	0.42666001E+04	0.53088447E-05
0.31531001E+04	0.55718519E-05	0.42851001E+04	0.53333501E-05
0.31722000E+04	0.55975765E-05	0.43036001E+04	0.53456424E-05
0.31907000E+04	0.55847045E-05	0.43221001E+04	0.53333501E-05
0.32092000E+04	0.55590394E-05	0.43406001E+04	0.53703175E-05
0.32277000E+04	0.55462560E-05	0.43591001E+04	0.53333501E-05
0.32462000E+04	0.55207729E-05	0.43783999E+04	0.53456424E-05
0.32647000E+04	0.55590394E-05	0.43963999E+04	0.53333501E-05
0.32832000E+04	0.55462560E-05	0.44153999E+04	0.52966320E-05
0.33017000E+04	0.55590394E-05	0.44338999E+04	0.52966320E-05
0.33202000E+04	0.55335026E-05	0.44523999E+04	0.52966320E-05
0.33387000E+04	0.55207729E-05	0.44708999E+04	0.52601717E-05
0.33572000E+04	0.55462560E-05	0.44893999E+04	0.52844525E-05
0.33757000E+04	0.55207729E-05	0.45078999E+04	0.52844525E-05
0.33942000E+04	0.5571851[illegible]-05	0.45263999E+04	0.53088447E-05

Table B-5 (continued)

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.45448999E+04	0.53068447E-05
0.45633999E+04	0.53210811E-05
0.45818999E+04	0.52601717E-05
0.46003999E+04	0.52844525E-05
0.46195000E+04	0.52360028E-05
0.46380000E+04	0.52360028E-05
0.46565000E+04	0.52601717E-05
0.46750000E+04	0.52844525E-05
0.46935000E+04	0.52844525E-05
0.47120000E+04	0.52966320E-05
0.47305000E+04	0.52480709E-05
0.47490000E+04	0.52480709E-05
0.47675000E+04	0.52239625E-05
0.47860000E+04	0.52239625E-05
0.48045000E+04	0.52239625E-05
0.48230000E+04	0.52360028E-05
0.48415000E+04	0.52601717E-05
0.48600000E+04	0.52966320E-05
0.48791001E+04	0.52480709E-05
0.48976001E+04	0.52239625E-05
0.49161001E+04	0.51880024E-05
0.49346001E+04	0.51999600E-05
0.49531001E+04	0.51999600E-05
0.49716001E+04	0.51999600E-05
0.49901001E+04	0.52119449E-05
0.50086001E+04	0.52239625E-05
0.50271001E+04	0.52119449E-05
0.50456001E+04	0.51880024E-05
0.50641001E+04	0.51522852E-05
0.50826001E+04	0.51641605E-05
0.51011001E+04	0.51404372E-05
0.51203999E+04	0.51404372E-05
0.51388999E+04	0.51760676E-05
0.51573999E+04	0.51760676E-05
0.51758999E+04	0.52119449E-05
0.51943999E+04	0.51760676E-05
0.52128999E+04	0.51999600E-05
0.52313999E+04	0.51286120E-05
0.52498999E+04	0.51760676E-05
0.52683999E+04	0.51641605E-05
0.52868999E+04	0.51286120E-05
0.53053999E+04	0.51286120E-05
0.53238999E+04	0.51286120E-05
0.53423999E+04	0.51404372E-05
0.53617002E+04	0.51404372E-05
0.53802002E+04	0.51404372E-05
0.53987002E+04	0.51522852E-05

Table B-5 (continued)

(b) Cell Two

Time (sec)	$[H^+]$ (M)
0.41799998E+01	0.24322032E-05
0.22680000E+02	0.64416895E-05
0.41180000E+02	0.12359477E-04
0.59680000E+02	0.18278048E-04
0.78180000E+02	0.24888570E-04
0.96680000E+02	0.31622763E-04
0.11520000E+03	0.37931506E-04
0.13380000E+03	0.44874512E-04
0.15270000E+03	0.51168212E-04
0.17120000E+03	0.56754459E-04
0.18970000E+03	0.63241219E-04
0.20820000E+03	0.69502406E-04
0.22670000E+03	0.74989446E-04
0.24520000E+03	0.80537829E-04
0.26370001E+03	0.85703788E-04
0.28220001E+03	0.90573223E-04
0.30070001E+03	0.94623654E-04
0.31920001E+03	0.99999990E-04
0.33770001E+03	0.10471287E-03
0.35620001E+03	0.10914406E-03
0.37500000E+03	0.11323997E-03
0.39379999E+03	0.11721952E-03
0.41229999E+03	0.12022645E-03
0.43079999E+03	0.12302684E-03
0.44929999E+03	0.12589246E-03
0.46779999E+03	0.12912187E-03
0.48629999F+03	0.13212959E-03
0.50479999E+03	0.13458599E-03
0.52329999E+03	0.13835657E-03
0.54179999E+03	0.14125383E-03
0.56029999E+03	0.14487715E-03
0.57879999E+03	0.14757055E-03
0.59729999E+03	0.14893619E-03
0.61620001E+03	0.15205469E-03
0.63520001E+03	0.15381553E-03
0.65370001E+03	0.15488168E-03
0.67220001E+03	0.15703635E-03
0.69070001E+03	0.15885457E-03
0.70920001E+03	0.15995580E-03
0.72770001E+03	0.16255488E-03
0.74620001E+03	0.16405886E-03
0.76470001E+03	0.16595870E-03
0.78320001E+03	0.16672460E-03
0.80170001E+03	0.16672460E-03
0.82020001E+03	0.16826748E-03
0.83870001E+03	0.16943380E-03
0.85720001E+03	0.17021573E-03
0.87590002E+03	0.17179076E-03
0.89479999E+03	0.17218688E-03
0.91329999E+03	0.17218688E-03
0.93179999E+03	0.17338037E-03
0.95029999E+03	0.17338037E-03
0.96879999E+03	0.17498467E-03
0.98729999E+03	0.17538799E-03
0.10060000E+04	0.17619756E-03
0.10240000E+04	0.17701088E-03
0.10430000E+04	0.17823781E-03
0.10610000E+04	0.17864878E-03
0.10800000E+04	0.17782794E-03
0.10980000E+04	0.17864878E-03
0.11170000E+04	0.18030184E-03
0.11360000E+04	0.17947324E-03
0.11550000E+04	0.17968707E-03
0.11730000E+04	0.18113393E-03
0.11920000E+04	0.18238943E-03
0.12100000E+04	0.18155159E-03
0.12290000E+04	0.18197003E-03
0.12470000E+04	0.18280998E-03
0.12660000E+04	0.18238943E-03
0.12840000E+04	0.18323150E-03
0.13030000E+04	0.18280998E-03
0.13210000E+04	0.18280998E-03
0.13400000E+04	0.18323150E-03
0.13580000E+04	0.18492679E-03
0.13770000E+04	0.18365381E-03
0.13960000E+04	0.18280998E-03
0.14140000E+04	0.18323150E-03
0.14330000E+04	0.18280998E-03
0.14510000E+04	0.18197003E-03
0.14700000E+04	0.18323150E-03
0.14880000E+04	0.18323150E-03
0.15070000E+04	0.18450155E-03
0.15250000E+04	0.18450155E-03
0.15440000E+04	0.18492679E-03
0.15620000E+04	0.18450155E-03
0.15810000E+04	0.18407729E-03
0.16000000E+04	0.18535301E-03
0.16190000E+04	0.18492679E-03
0.16370000E+04	0.18706829E-03
0.16560000E+04	0.18578040E-03
0.16740000E+04	0.18578040E-03
0.16930000E+04	0.18450155E-03
0.17110000E+04	0.18578040E-03
0.17290000E+04	0.18620877E-03
0.17480000E+04	0.18578040E-03
0.17660000E+04	0.18578040E-03
0.17850000E+04	0.18578040E-03
0.18030000E+04	0.18620877E-03
0.18220000E+04	0.18620877E-03
0.18410000E+04	0.18492679E-03
0.18600000E+04	0.18535301E-03
0.18780000E+04	0.18535301E-03
0.18970000E+04	0.18492679E-03
0.19150000E+04	0.18535301E-03
0.19340000E+04	0.18578040E-03
0.19520000E+04	0.18620877E-03
0.19710000E+04	0.18535301E-03
0.19890000E+04	0.18578040E-03
0.20080000E+04	0.18663795E-03
0.20260000E+04	0.18620877E-03
0.20450000E+04	0.18578040E-03
0.20630000E+04	0.18706829E-03
0.20820000E+04	0.18706829E-03
0.21010000E+04	0.18535301E-03
0.21190000E+04	0.18706829E-03
0.21380000E+04	0.18578040E-03
0.21560000E+04	0.18749945E-03
0.21750000E+04	0.18620877E-03
0.21930000E+04	0.18620877E-03
0.22120000E+04	0.18620877E-03
0.22300000E+04	0.18578040E-03
0.22490000E+04	0.18578040E-03

Table B-5 (continued)

(b) Cell Two

Time (sec)	$[H^+]$ (M)	Time (sec)	$[H^+]$ (M)
0.22670000E+04	0.18535301E-03	0.33990000E+04	0.18578040E-03
0.22860000E+04	0.18492679E-03	0.34180000E+04	0.18450155E-03
0.23040000E+04	0.18492679E-03	0.34360000E+04	0.18578040E-03
0.23230000E+04	0.18578040E-03	0.34550000E+04	0.18450155E-03
0.23420000E+04	0.18663795E-03	0.34730000E+04	0.18492679E-03
0.23600000E+04	0.18793160E-03	0.34920000E+04	0.18407729E-03
0.23790000E+04	0.18793160E-03	0.35100000E+04	0.18535301E-03
0.23970000E+04	0.18706829E-03	0.35290000E+04	0.18450155E-03
0.24160000E+04	0.18620877E-03	0.35470000E+04	0.18450155E-03
0.24340000E+04	0.18663795E-03	0.35660000E+04	0.18450155E-03
0.24530000E+04	0.18706829E-03	0.35850000E+04	0.18407729E-03
0.24710000E+04	0.18663795E-03	0.36030000E+04	0.18450155E-03
0.24900000E+04	0.18663795E-03	0.36220000E+04	0.18450155E-03
0.25080000E+04	0.18663795E-03	0.36400000E+04	0.18450155E-03
0.25270000E+04	0.18578040E-03	0.36590000E+04	0.18450155E-03
0.25450000E+04	0.18578040E-03	0.36770000E+04	0.18492679E-03
0.25640000E+04	0.18492679E-03	0.36960000E+04	0.18492679E-03
0.25830000E+04	0.18492679E-03	0.37140000E+04	0.18535301E-03
0.26020000E+04	0.18578040E-03	0.37330000E+04	0.18450155E-03
0.26200000E+04	0.18620877E-03	0.37510000E+04	0.18706829E-03
0.26390000E+04	0.18535301E-03	0.37700000E+04	0.18535301E-03
0.26570000E+04	0.18450155E-03	0.37890000E+04	0.18450155E-03
0.26760000E+04	0.18450155E-03	0.38070000E+04	0.18535301E-03
0.26940000E+04	0.18323150E-03	0.38260000E+04	0.18450155E-03
0.27130000E+04	0.18407729E-03	0.38440000E+04	0.18492679E-03
0.27310000E+04	0.18492679E-03	0.38630000E+04	0.18407729E-03
0.27500000E+04	0.18578040E-03	0.38810000E+04	0.18450155E-03
0.27680000E+04	0.18620877E-03	0.39000000E+04	0.18535301E-03
0.27870000E+04	0.18620877E-03	0.39180000E+04	0.18535301E-03
0.28050000E+04	0.18620877E-03	0.39370000E+04	0.18535301E-03
0.28240000E+04	0.18663795E-03	0.39550000E+04	0.18535301E-03
0.28430000E+04	0.18578040E-03	0.39740000E+04	0.18323150E-03
0.28610000E+04	0.18620877E-03	0.39920000E+04	0.18407729E-03
0.28800000E+04	0.18578040E-03	0.40110000E+04	0.18407729E-03
0.28980000E+04	0.18578040E-03	0.40300000E+04	0.18365381E-03
0.29170000E+04	0.18578040E-03	0.40490000E+04	0.18450155E-03
0.29350000E+04	0.18535301E-03	0.40670000E+04	0.18492679E-03
0.29540000E+04	0.18492679E-03	0.40860000E+04	0.18535301E-03
0.29720000E+04	0.18663795E-03	0.41040000E+04	0.18492679E-03
0.29910000E+04	0.18535301E-03	0.41230000E+04	0.18535301E-03
0.30090000E+04	0.18578040E-03	0.41410000E+04	0.18535301E-03
0.30280000E+04	0.18578040E-03	0.41600000E+04	0.18407729E-03
0.30460000E+04	0.18492679E-03	0.41780000E+04	0.18535301E-03
0.30650000E+04	0.18620877E-03	0.41970000E+04	0.18450155E-03
0.30840000E+04	0.18620877E-03	0.42150000E+04	0.18492679E-03
0.31020000E+04	0.18492679E-03	0.42340000E+04	0.18492679E-03
0.31210000E+04	0.18450155E-03	0.42520000E+04	0.18578040E-03
0.31390000E+04	0.18450155E-03	0.42710000E+04	0.18492679E-03
0.31580000E+04	0.18492679E-03	0.42900000E+04	0.18450155E-03
0.31760000E+04	0.18535301E-03	0.43080000E+04	0.18450155E-03
0.31950000E+04	0.18450155E-03	0.43270000E+04	0.18407729E-03
0.32130000E+04	0.18535301E-03	0.43450000E+04	0.18450155E-03
0.32320000E+04	0.18535301E-03	0.43640000E+04	0.18407729E-03
0.32500000E+04	0.18535301E-03	0.43820000E+04	0.18450155E-03
0.32690000E+04	0.18620877E-03	0.44010000E+04	0.18280998E-03
0.32870000E+04	0.18578040E-03	0.44190000E+04	0.18280998E-03
0.33060000E+04	0.18450155E-03	0.44380000E+04	0.18450155E-03
0.33250000E+04	0.18578040E-03	0.44560000E+04	0.18450155E-03
0.33440000E+04	0.18535301E-03	0.44750000E+04	0.18535301E-03
0.33620000E+04	0.18535301E-03	0.44930000E+04	0.18578040E-03
0.33810000E+04	0.18450155E-03	0.45120000E+04	0.18492679E-03

Table B-5 (concluded)

(b) Cell Two

Time (sec)	$[H^+]$ (M)
0.45310000E+04	0.18492679E-03
0.45500000E+04	0.18450155E-03
0.45680000E+04	0.18450155E-03
0.45870000E+04	0.18492679E-03
0.46050000E+04	0.18450155E-03
0.46240000E+04	0.18450155E-03
0.46420000E+04	0.18535301E-03
0.46610000E+04	0.18492679E-03
0.46790000E+04	0.18450155E-03
0.46980000E+04	0.18365381E-03
0.47160000E+04	0.18450155E-03
0.47340000E+04	0.18450155E-03
0.47530000E+04	0.18492679E-03
0.47720000E+04	0.18450155E-03
0.47910000E+04	0.18450155E-03
0.48090000E+04	0.18407729E-03
0.48280000E+04	0.18492679E-03
0.48460000E+04	0.18365381E-03
0.48650000E+04	0.18450155E-03
0.48830000E+04	0.18492679E-03
0.49020000E+04	0.18492679E-03
0.49200000E+04	0.18450155E-03
0.49390000E+04	0.18450155E-03
0.49570000E+04	0.18535301E-03
0.49760000E+04	0.18365381E-03
0.49940000E+04	0.18492679E-03
0.50130000E+04	0.18492679E-03
0.50320000E+04	0.18535301E-03
0.50500000E+04	0.18450155E-03
0.50690000E+04	0.18535301E-03
0.50870000E+04	0.18535301E-03
0.51060000E+04	0.18578040E-03
0.51240000E+04	0.18535301E-03
0.51430000E+04	0.18365381E-03
0.51610000E+04	0.18407729E-03
0.51800000E+04	0.18450155E-03
0.51980000E+04	0.18280998E-03
0.52170000E+04	0.18407729E-03
0.52350000E+04	0.18365381E-03
0.52540000E+04	0.18407729E-03
0.52730000E+04	0.18492679E-03
0.52920000E+04	0.18450155E-03

Table B-6

Data for Mustard Hydrolysis at 308 K

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.18690001E+02	0.20558916E-05
0.37180000E+02	0.10789467E-04
0.55660000E+02	0.23280923E-04
0.74169998E+02	0.35481335E-04
0.92660004E+02	0.47533500E-04
0.11115000E+03	0.58479029E-04
0.12964000E+03	0.68076974E-04
0.14813000E+03	0.76032607E-04
0.16663000E+03	0.85506712E-04
0.18512000E+03	0.91201109E-04
0.20361000E+03	0.98401106E-04
0.22211000E+03	0.10115792E-03
0.24059999E+03	0.10859299E-03
0.25942001E+03	0.11015389E-03
0.27792001E+03	0.11534551E-03
0.29641000E+03	0.11694997E-03
0.31489999E+03	0.12022645E-03
0.33339999E+03	0.12105978E-03
0.35189001E+03	0.12387958E-03
0.37038000E+03	0.12416522E-03
0.38888000E+03	0.12676518E-03
0.40737000E+03	0.12676515E-03
0.42585999E+03	0.12912157E-03
0.44435999E+03	0.12793817E-03
0.46285001E+03	0.12971788E-03
0.48201001E+03	0.12971788E-03
0.50050000E+03	0.13061702E-03
0.51900000E+03	0.13061702E-03
0.53748999E+03	0.13152249E-03
0.55597998E+03	0.13031665E-03
0.57447998E+03	0.13212959E-03
0.59296997E+03	0.13031665E-03
0.61146997E+03	0.13212959E-03
0.62996002E+03	0.13182563E-03
0.64846002E+03	0.13304543E-03
0.66695001E+03	0.13091818E-03
0.68545001E+03	0.13335208E-03
0.70394000E+03	0.13091818E-03
0.72309998E+03	0.13335208E-03
0.74159003E+03	0.13091818E-03
0.76009003E+03	0.13273935E-03
0.77858002E+03	0.13061702E-03
0.79707001E+03	0.13304543E-03
0.81557001E+03	0.13121993E-03
0.83407001E+03	0.13304543E-03
0.85256000E+03	0.13121993E-03
0.87104999E+03	0.13335208E-03
0.88954999E+03	0.13152249E-03
0.90803998E+03	0.13152249E-03
0.92653003E+03	0.13182563E-03
0.94503003E+03	0.13152249E-03
0.96352002E+03	0.13182563E-03
0.98251001E+03	0.13091818E-03
0.10010000E+04	0.13212959E-03
0.10195000E+04	0.13061702E-03
0.10380000E+04	0.13243413E-03
0.10565000E+04	0.13001698E-03
0.10750000E+04	0.13182563E-03
0.10935000E+04	0.13031665E-03
0.11120000E+04	0.13152249E-03
0.11305000E+04	0.12971788E-03
0.11490000E+04	0.13182563E-03
0.11675000E+04	0.13031665E-03
0.11860000E+04	0.13061702E-03
0.12044000E+04	0.13061702E-03
0.12236000E+04	0.13121993E-03
0.12421000E+04	0.13001698E-03
0.12606000E+04	0.13061702E-03
0.12791000E+04	0.13121993E-03
0.12976000E+04	0.13001698E-03
0.13161000E+04	0.13121993E-03
0.13346000E+04	0.12912187E-03
0.13531000E+04	0.13152249E-03
0.13716000E+04	0.12941960E-03
0.13901000E+04	0.13061702E-03
0.14086000E+04	0.12971788E-03
0.14270000E+04	0.13001698E-03
0.14455000E+04	0.13031665E-03
0.14647000E+04	0.12882495E-03
0.14832000E+04	0.13091818E-03
0.15017000E+04	0.12941960E-03
0.15202000E+04	0.13061702E-03
0.15387000E+04	0.12882495E-03
0.15572000E+04	0.12971788E-03
0.15757000E+04	0.12971788E-03
0.15942000E+04	0.12852860E-03
0.16127000E+04	0.13121993E-03
0.16312000E+04	0.12823303E-03
0.16497000E+04	0.13001698E-03
0.16681000E+04	0.12882495E-03
0.16866000E+04	0.12941960E-03
0.17056000E+04	0.12912187E-03
0.17241000E+04	0.12912187E-03
0.17426000E+04	0.12971788E-03
0.17611000E+04	0.12793817E-03
0.17796000E+04	0.13061702E-03
0.17981000E+04	0.12852860E-03
0.18166000E+04	0.13001698E-03
0.18351000E+04	0.12912187E-03
0.18536000E+04	0.12941960E-03
0.18721000E+04	0.13001698E-03
0.18906000E+04	0.12764364E-03
0.19091000E+04	0.12971788E-03
0.19276000E+04	0.12852860E-03
0.19467000E+04	0.12852860E-03
0.19652000E+04	0.12912187E-03
0.19837000E+04	0.12793817E-03
0.20022000E+04	0.13001698E-03
0.20207000E+04	0.12764384E-03
0.20392000E+04	0.12852860E-03
0.20577000E+04	0.12971788E-03
0.20762000E+04	0.12735053E-03
0.20947000E+04	0.12941960E-03
0.21132000E+04	0.12764384E-03
0.21317000E+04	0.12852860E-03
0.21502000E+04	0.12912187E-03
0.21687000E+04	0.12764384E-03
0.21877000E+04	0.12971788E-03
0.22062000E+04	0.12793817E-03
0.22247000E+04	0.12882495E-03
0.22431001E+04	0.12882495E-03
0.22616001E+04	0.12764384E-03

Table B-6 (continued)

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.22801001E+04	0.12912187E-03
0.22986001E+04	0.12764384E-03
0.23171001E+04	0.12764384E-03
0.23356001E+04	0.12852860E-03
0.23541001E+04	0.12705749E-03
0.23726001E+04	0.12912187E-03
0.23911001E+04	0.12852860E-03
0.24096001E+04	0.12735033E-03
0.24286001E+04	0.12882495E-03
0.24471001E+04	0.12735033E-03
0.24656001E+04	0.12735033E-03
0.24841001E+04	0.12882495E-03
0.25026001E+04	0.12823303E-03
0.25211001E+04	0.12705749E-03
0.25395000E+04	0.12882495E-03
0.25580000E+04	0.12764384E-03
0.25765000E+04	0.12676518E-03
0.25950000E+04	0.12882495E-03
0.26135000E+04	0.12735033E-03
0.26320000E+04	0.12676518E-03
0.26505000E+04	0.12823303E-03
0.26697000E+04	0.12676518E-03
0.26882000E+04	0.12647356E-03
0.27067000E+04	0.12852860E-03
0.27252000E+04	0.12764384E-03
0.27437000E+04	0.12647356E-03
0.27622000E+04	0.12764384E-03
0.27806001E+04	0.12823303E-03
0.27991001E+04	0.12676518E-03
0.28176001E+04	0.12676518E-03
0.28361001E+04	0.12882495E-03
0.28546001E+04	0.12618274E-03
0.28731001E+04	0.12705749E-03
0.28916001E+04	0.12823303E-03
0.29101001E+04	0.12647356E-03
0.29291001E+04	0.12676518E-03
0.29476001E+04	0.12823303E-03
0.29661001E+04	0.12647356E-03
0.29846001E+04	0.12589246E-03
0.30031001E+04	0.12735033E-03
0.30216001E+04	0.12676518E-03
0.30401001E+04	0.12618274E-03
0.30586001E+04	0.12735033E-03
0.30771001E+04	0.12676518E-03
0.30956001E+04	0.12560296E-03
0.31141001E+04	0.12764384E-03
0.31326001E+04	0.12735033E-03
0.31511001E+04	0.12647356E-03
0.31702000E+04	0.12764384E-03
0.31887000E+04	0.12735033E-03
0.32072000E+04	0.12618274E-03
0.32257000E+04	0.12647356E-03
0.32442000E+04	0.12764384E-03
0.32627000E+04	0.12618274E-03
0.32812000E+04	0.12589246E-03
0.32997000E+04	0.12705749E-03
0.33182000E+04	0.12705749E-03
0.33367000E+04	0.12589246E-03
0.33552000E+04	0.12618274E-03
0.33737000E+04	0.12735033E-03
0.33922000E+04	0.12502586E-03
0.34113000E+04	0.12618274E-03
0.34298000E+04	0.12735033E-03
0.34483000E+04	0.12589246E-03
0.34668000E+04	0.12502586E-03
0.34853000E+04	0.12676518E-03
0.35038000E+04	0.12589246E-03
0.35223000E+04	0.12502586E-03
0.35408000E+04	0.12647356E-03

Table B-6 (continued)

(b) Cell Two

Time (sec)	[H^+] (M)
0.41199999E+01	0.35892196E-07
0.22610001E+02	0.63386972E-06
0.41099998E+02	0.57544039E-05
0.59590000E+02	0.19906716E-04
0.78089996E+02	0.34276756E-04
0.96580002E+02	0.49090762E-04
0.11510000E+03	0.62373489E-04
0.13370000E+03	0.74473239E-04
0.15239999E+03	0.89949746E-04
0.17089999E+03	0.98401106E-04
0.18939999E+03	0.10739888E-03
0.20789999E+03	0.11508007E-03
0.22639999E+03	0.11912418E-03
0.24489999E+03	0.13001698E-03
0.26339999E+03	0.13121993E-03
0.28179999E+03	0.13803842E-03
0.30029999E+03	0.14060468E-03
0.31879999E+03	0.14621772E-03
0.33729999E+03	0.14554590E-03
0.35579999E+03	0.15100800E-03
0.37470001E+03	0.15170504E-03
0.39350000E+03	0.15595522E-03
0.41200000E+03	0.15488168E-03
0.43050000E+03	0.15595522E-03
0.44900000E+03	0.15739830E-03
0.46739999E+03	0.15776107E-03
0.48589999E+03	0.15739830E-03
0.50439999E+03	0.15995580E-03
0.52290002E+03	0.15848929E-03
0.54140002E+03	0.15958799E-03
0.55990002E+03	0.15885457E-03
0.57840002E+03	0.16255488E-03
0.59690002E+03	0.16069415E-03
0.61579999E+03	0.16032447E-03
0.63459998E+03	0.16106453E-03
0.65300000E+03	0.16218108E-03
0.67150000E+03	0.16443714E-03
0.69000000E+03	0.16443714E-03
0.70850000E+03	0.16368160E-03
0.72700000E+03	0.16368160E-03
0.74550000E+03	0.16106453E-03
0.76400000E+03	0.16255488E-03
0.78250000E+03	0.16557708E-03
0.80100000E+03	0.16519616E-03
0.81950000E+03	0.16292953E-03
0.83800000E+03	0.16330522E-03
0.85650000E+03	0.16557708E-03
0.87529999E+03	0.16405886E-03
0.89400000E+03	0.16481630E-03
0.91250000E+03	0.16443714E-03
0.93100000E+03	0.16405886E-03
0.94950000E+03	0.16368160E-03
0.96500000E+03	0.16368160E-03
0.98640002E+03	0.16443714E-03
0.10050000E+04	0.16519616E-03
0.10230000E+04	0.16481630E-03
0.10420000E+04	0.16519616E-03
0.10600000E+04	0.16292953E-03
0.10790000E+04	0.16519616E-03
0.10970000E+04	0.16218108E-03
0.11160000E+04	0.16443714E-03

Time (sec)	[H^+] (M)
0.11350000E+04	0.16405886E-03
0.11540000E+04	0.16292953E-03
0.11720000E+04	0.16330522E-03
0.11910000E+04	0.16218108E-03
0.12090000E+04	0.16255488E-03
0.12280000E+04	0.16255488E-03
0.12460000E+04	0.16292953E-03
0.12650000E+04	0.16032447E-03
0.12830000E+04	0.16255488E-03
0.13020000E+04	0.16218108E-03
0.13200000E+04	0.15995580E-03
0.13390000E+04	0.16368160E-03
0.13570000E+04	0.16218108E-03
0.13760000E+04	0.16106453E-03
0.13950000E+04	0.16143575E-03
0.14130000E+04	0.16180798E-03
0.14320000E+04	0.15995580E-03
0.14500000E+04	0.16106453E-03
0.14690000E+04	0.16180798E-03
0.14870000E+04	0.16069415E-03
0.15060000E+04	0.16069415E-03
0.15240000E+04	0.16106453E-03
0.15430000E+04	0.16106453E-03
0.15610000E+04	0.16069415E-03
0.15800000E+04	0.16069415E-03
0.15980000E+04	0.16180798E-03
0.16170000E+04	0.16255488E-03
0.16360000E+04	0.16405886E-03
0.16540000E+04	0.16032447E-03
0.16730000E+04	0.16180798E-03
0.16910000E+04	0.16069415E-03
0.17100000E+04	0.16481630E-03
0.17280000E+04	0.16069415E-03
0.17470000E+04	0.16218108E-03
0.17650000E+04	0.16106453E-03
0.17840000E+04	0.16032447E-03
0.18020000E+04	0.16032447E-03
0.18210000E+04	0.16143575E-03
0.18400000E+04	0.15958799E-03
0.18580000E+04	0.16106453E-03
0.18770000E+04	0.16032447E-03
0.18950000E+04	0.16255488E-03
0.19140000E+04	0.16106453E-03
0.19320000E+04	0.16180798E-03
0.19510000E+04	0.16106453E-03
0.19690000E+04	0.16143575E-03
0.19880000E+04	0.16218108E-03
0.20060000E+04	0.16255488E-03
0.20250000E+04	0.16180798E-03
0.20430000E+04	0.16292953E-03
0.20620000E+04	0.15885457E-03
0.20810000E+04	0.16032447E-03
0.20990000E+04	0.15922086E-03
0.21180000E+04	0.16218108E-03
[illegible]360000E+04	0.16218108E-03
[illegible]550000E+04	0.[illegible]032447E-03
[illegible]1730000E+04	0.16292953E-03
0.21920000E+04	0.16143575E-03
0.22100000E+04	0.16143575E-03
0.22290000E+04	0.16218108E-03
0.22470000E+04	0.16180798E-03

Table B-6 (concluded)

(b) Cell Two

Time (sec)	$[H^+]$ (M)
0.22660000E+04	0.16255488E-03
0.22840000E+04	0.16255488E-03
0.23030000E+04	0.16069415E-03
0.23210000E+04	0.16255488E-03
0.23400000E+04	0.16218108E-03
0.23590000E+04	0.16180798E-03
0.23770000E+04	0.16330522E-03
0.23960000E+04	0.16368160E-03
0.24140000E+04	0.16255488E-03
0.24330000E+04	0.16368160E-03
0.24510000E+04	0.16330522E-03
0.24700000E+04	0.16218108E-03
0.24880000E+04	0.16405886E-03
0.25070000E+04	0.16255488E-03
0.25250000E+04	0.16143575E-03
0.25440000E+04	0.16443714E-03
0.25620000E+04	0.16405886E-03
0.25810000E+04	0.16368160E-03
0.26000000E+04	0.16443714E-03
0.26180000E+04	0.16368160E-03
0.26370000E+04	0.16255488E-03
0.26550000E+04	0.16368160E-03
0.26740000E+04	0.16405886E-03
0.26920000E+04	0.16218108E-03
0.27110000E+04	0.16443714E-03
0.27290000E+04	0.16292953E-03
0.27480000E+04	0.16292953E-03
0.27660000E+04	0.16330522E-03
0.27850000E+04	0.16405886E-03
0.28030000E+04	0.16255488E-03
0.28220000E+04	0.16292953E-03
0.28410000E+04	0.16481630E-03
0.28590000E+04	0.16218108E-03
0.28780000E+04	0.16255488E-03
0.28960000E+04	0.16368160E-03
0.29150000E+04	0.16218108E-03
0.29330000E+04	0.16292953E-03
0.29520000E+04	0.16330522E-03
0.29700000E+04	0.16180798E-03
0.29890000E+04	0.16032447E-03
0.30070000E+04	0.16255488E-03
0.30260000E+04	0.16180798E-03
0.30440000E+04	0.16180798E-03
0.30630000E+04	0.16069415E-03
0.30820000E+04	0.16218108E-03
0.31000000E+04	0.16292953E-03
0.31190000E+04	0.16292953E-03
0.31370000E+04	0.15922086E-03
0.31560000E+04	0.16330522E-03
0.31740000E+04	0.16255488E-03
0.31930000E+04	0.16368160E-03
0.32110000E+04	0.16218108E-03
0.32300000E+04	0.16143575E-03
0.32480000E+04	0.16292953E-03
0.32670000E+04	0.16218108E-03
0.32850000E+04	0.16292953E-03
0.33040000E+04	0.16180798E-03
0.33230000E+04	0.16368160E-03
0.33410000E+04	0.16069415E-03
0.33600000E+04	0.16368160E-03
0.33780000E+04	0.16180798E-03
0.33970000E+04	0.16443714E-03
0.34150000E+04	0.16368160E-03
0.34340000E+04	0.16595870E-03
0.34520000E+04	0.16519616E-03
0.34710000E+04	0.16292953E-03
0.34890000E+04	0.16255488E-03
0.35080000E+04	0.16218108E-03
0.35260000E+04	0.16106453E-03

Table B-7

Data for Mustard Hydrolysis at 313 K

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.18700001E+02	0.42953607E-05
0.37189999E+02	0.20749121E-04
0.55689999E+02	0.38815069E-04
0.74190002E+02	0.55335000E-04
0.92690002E+02	0.69662601E-04
0.11118000E+03	0.79983358E-04
0.12967999E+03	0.89742905E-04
0.14817999E+03	0.96161159E-04
0.16667000E+03	0.10303863E-03
0.18517000E+03	0.10864258E-03
0.20367000E+03	0.11142939E-03
0.22217000E+03	0.11297957E-03
0.24117000E+03	0.11776060E-03
0.25966000E+03	0.11912419E-03
0.27316000E+03	0.11939873E-03
0.29666000E+03	0.12105978E-03
0.31514999E+03	0.12359473E-03
0.33364999E+03	0.12246157E-03
0.35214999E+03	0.12189839E-03
0.37064999E+03	0.12387958E-03
0.38914999E+03	0.12502586E-03

Table B-7 (concluded)

(b) Cell Two

Time (sec)	$[H^+]$ (M)
0.20160000E+02	0.69183095E-07
0.38660000E+02	0.72945745E-07
0.57150002E+02	0.72443541E-07
0.75650002E+02	0.69984182E-07
0.94150002E+02	0.69502370E-07
0.11264000E+03	0.81846457E-06
0.13114000E+03	0.15452544E-04
0.14964000E+03	0.40738018E-04
0.16813000E+03	0.64268803E-04
0.18663000E+03	0.86496737E-04
0.20513000E+03	0.10471287E-03
0.22384000E+03	0.11912418E-03
0.24263000E+03	0.13304543E-03
0.26112000E+03	0.14223291E-03
0.27962000E+03	0.15812469E-03
0.29812000E+03	0.15922086E-03
0.31660999E+03	0.16405886E-03
0.33510999E+03	0.17060821E-03
0.35360999E+03	0.17378014E-03
0.37210999E+03	0.17579223E-03
0.39060001E+03	0.17498467E-03

Table B-8

Data for Mustard Hydrolysis at 318 K

(a) Cell One

Time (sec)	$[H^+]$ (M)
0.18700001E+02	0.12133865E-04
0.37200001E+02	0.44157023E-04
0.55700001E+02	0.72443561E-04
0.74199997E+02	0.93756207E-04
0.92690002E+02	0.10864258E-03
0.11119000E+03	0.11994987E-03
0.12969000E+03	0.12764384E-03
0.14819000E+03	0.13335208E-03
0.16669000E+03	0.13677284E-03
0.18517999E+03	0.13963657E-03
0.20367999E+03	0.14157940E-03
0.22217999E+03	0.14228932E-03
0.24117999E+03	0.14387986E-03
0.25967999E+03	0.14487715E-03
0.27817001E+03	0.14554590E-03
0.29667001E+03	0.14588149E-03
0.31517001E+03	0.14621772E-03
0.33367001E+03	0.14621772E-03
0.35217001E+03	0.14588149E-03
0.37067001E+03	0.14689265E-03
0.38917001E+03	0.14621772E-03
0.40767999E+03	0.14588149E-03
0.42617001E+03	0.14588149E-03
0.44467001E+03	0.14521107E-03
0.46317001E+03	0.14521107E-03
0.48234000E+03	0.14521107E-03
0.50084000E+03	0.14421149E-03
0.51934003E+03	0.14454400E-03
0.53784003E+03	0.14387986E-03
0.55634003E+03	0.14454400E-03
0.57484003E+03	0.14454400E-03
0.59334998E+03	0.14454400E-03
0.61184998E+03	0.14521107E-03
0.63034998E+03	0.14554590E-03
0.64884998E+03	0.14621772E-03
0.66734998E+03	0.14621772E-03
0.68584998E+03	0.14723121E-03
0.70435999E+03	0.14689265E-03
0.72353003E+03	0.14689265E-03
0.74203003E+03	0.14655472E-03
0.76053003E+03	0.14621772E-03
0.77903003E+03	0.14588149E-03
0.79753003E+03	0.14588149E-03
0.81603998E+03	0.14588149E-03
0.83453998E+03	0.14487715E-03
0.85303998E+03	0.14521107E-03
0.87153998E+03	0.14454400E-03
0.89003998E+03	0.14454400E-03
0.90853998E+03	0.14521107E-03
0.92703998E+03	0.14454400E-03
0.94553998E+03	0.14421149E-03
0.96403998E+03	0.14421149E-03
0.98303998E+03	0.14387986E-03
0.10015000E+04	0.14454400E-03
0.10201000E+04	0.14454400E-03
0.10386000E+04	0.14454400E-03
0.10571000E+04	0.14521107E-03
0.10756000E+04	0.14521107E-03
0.10941000E+04	0.14588149E-03
0.11126000E+04	0.14588149E-03
0.11311000E+04	0.14621772E-03
0.11496000E+04	0.14689265E-03
0.11681000E+04	0.14621772E-03
0.11866000E+04	0.14655472E-03
0.12051000E+04	0.14588149E-03
0.12242000E+04	0.14554590E-03
0.12427000E+04	0.14554590E-03
0.12613000E+04	0.14487715E-03
0.12798000E+04	0.14421149E-03
0.12983000E+04	0.14421149E-03
0.13168000E+04	0.14454400E-03
0.13353000E+04	0.14454400E-03
0.13538000E+04	0.14454400E-03
0.13723000E+04	0.14521107E-03
0.13908000E+04	0.14554590E-03
0.14093000E+04	0.14655472E-03
0.14278000E+04	0.14655472E-03
0.14463000E+04	0.14621772E-03
0.14653000E+04	0.14588149E-03
0.14836000E+04	0.14554590E-03
0.15023000E+04	0.14521107E-03

Table B-8 (concluded)

(b) Cell Two

Time (sec)	$[H^+]$ (M)
0.20160000E+02	0.11748973E-06
0.38669998E+02	0.11748973E-06
0.57160000E+02	0.11967408E-06
0.75660004E+02	0.96382973E-06
0.94150002E+02	0.29922619E-04
0.11265000E+03	0.67297653E-04
0.13114999E+03	0.97949072E-04
0.14964999E+03	0.12050355E-03
0.16614000E+03	0.13489033E-03
0.18664000E+03	0.14757055E-03
0.20514000E+03	0.15667510E-03
0.22391000E+03	0.16106453E-03
0.24264000E+03	0.16519616E-03
0.26114001E+03	0.17021573E-03
0.27963000E+03	0.17139573E-03
0.29813000E+03	0.17100159E-03
0.31663000E+03	0.17458230E-03
0.33513000E+03	0.17458230E-03
0.35363000E+03	0.17579223E-03
0.37213000E+03	0.17498467E-03
0.39063000E+03	0.17418068E-03
0.40913000E+03	0.17619756E-03
0.42763000E+03	0.17538799E-03
0.44613000E+03	0.17660383E-03
0.46497000E+03	0.17823781E-03
0.48379999E+03	0.17538799E-03
0.50229999E+03	0.17741902E-03
0.52079999E+03	0.17701088E-03
0.53929999E+03	0.17701088E-03
0.55779999E+03	0.17619756E-03
0.57629999E+03	0.17458230E-03
0.59481000E+03	0.17823781E-03
0.61331000E+03	0.17538799E-03
0.63181000E+03	0.17619756E-03
0.65031000E+03	0.17701088E-03
0.66881000E+03	0.17579223E-03
0.68731000E+03	0.17418068E-03
0.70621997E+03	0.17498467E-03
0.72497998E+03	0.17579223E-03
0.74348999E+03	0.17378014E-03
0.76198999E+03	0.17579223E-03
0.78048999E+03	0.17458230E-03
0.79900000E+03	0.17538799E-03
0.81748999E+03	0.17498467E-03
0.83600000E+03	0.17418068E-03
0.85450000E+03	0.17823781E-03
0.87300000E+03	0.17741902E-03
0.89150000E+03	0.17619756E-03
0.91000000E+03	0.17947324E-03
0.92850000E+03	0.17741902E-03
0.94700000E+03	0.17538799E-03
0.96579999E+03	0.17864878E-03
0.98450000E+03	0.17538799E-03
0.10030000E+04	0.17579223E-03
0.10215000E+04	0.17538799E-03
0.10400000E+04	0.17619756E-03
0.10585000E+04	0.17498467E-03
0.10770000E+04	0.17538799E-03
0.10955000E+04	0.17458230E-03
0.11140000E+04	0.17258374E-03
0.11325000E+04	0.17579223E-03
0.11510000E+04	0.17458230E-03
0.11695000E+04	0.17579223E-03
0.11880000E+04	0.17579223E-03
0.12064000E+04	0.17579223E-03
0.12257000E+04	0.17458230E-03
0.12442000E+04	0.17619756E-03
0.12627000E+04	0.17782794E-03
0.12812000E+04	0.17538799E-03
0.12997000E+04	0.17619756E-03
0.13182000E+04	0.17741902E-03
0.13367000E+04	0.17579223E-03
0.13552000E+04	0.17660383E-03
0.13737000E+04	0.17498467E-03
0.13922000E+04	0.17378014E-03
0.14107000E+04	0.17619756E-03
0.14292000E+04	0.17378014E-03
0.14480000E+04	0.17579223E-03
0.14667000E+04	0.17458230E-03
0.14852000E+04	0.17538799E-03
0.15037000E+04	0.17418068E-03

Table B-9

Data for Mustard Hydrolysis at 298 K
and 0.05 Mole Fraction Ethanol

Time (sec)	$[H^+]$ (M)
0.18500000E+02	0.10256514E-06
0.37000000E+02	0.17338027E-06
0.55599998E+02	0.29512080E-06
0.74300003E+02	0.50118695E-06
0.92600003E+02	0.79799429E-06
0.11090000E+03	0.12823330E-05
0.13000000E+03	0.21777029E-05
0.14780000E+03	0.33419524E-05
0.16660001E+03	0.50234265E-05
0.18570000E+03	0.60221069E-05
0.20364999E+03	0.85113788E-05
0.22221001E+03	0.10665953E-04
0.24135001E+03	0.12331045E-04
0.25985999E+03	0.14791038E-04
0.27631000E+03	0.16557693E-04
0.29691000E+03	0.18535327E-04
0.31539001E+03	0.20323574E-04
0.33379999E+03	0.22594362E-04
0.35232001E+03	0.23985327E-04
0.37087000E+03	0.26121605E-04
0.38929001E+03	0.28313934E-04
0.40789001E+03	0.29174265E-04
0.42629999E+03	0.31695679E-04
0.44476999E+03	0.32734042E-04
0.46335999E+03	0.34753608E-04
0.48254999E+03	0.36307789E-04
0.50120001E+03	0.38904531E-04
0.51969000E+03	0.40271698E-04
0.53821002E+03	0.41399955E-04
0.55665997E+03	0.41975902E-04
0.57521002E+03	0.44157023E-04
0.59377002E+03	0.46344663E-04
0.61212000E+03	0.46238092E-04
0.63072998E+03	0.48417238E-04
0.64915002E+03	0.48565251E-04
0.66759998E+03	0.50118649E-04
0.68621997E+03	0.52601747E-04
0.70459003E+03	0.53703152E-04
0.72360999E+03	0.55080804E-04
0.74220001E+03	0.56885325E-04
0.76071997E+03	0.59156115E-04
0.77915002E+03	0.59703554E-04
0.79763000E+03	0.60255996E-04
0.81610999E+03	0.61517676E-04
0.83459998E+03	0.62086903E-04
0.85320001E+03	0.62373469E-04
0.87170001E+03	0.63095729E-04
0.89015002E+03	0.63973508E-04
0.90865997E+03	0.64563430E-04
0.92719000E+03	0.66069362E-04
0.94565997E+03	0.66580643E-04
0.96415997E+03	0.67452527E-04
0.98323003E+03	0.68546776E-04
0.10015000E+04	0.69342590E-04
0.10200000E+04	0.70631739E-04
0.10390000E+04	0.71779403E-04
0.10576000E+04	0.72110728E-04
0.10760000E+04	0.72276998E-04
0.10942000E+04	0.72443581E-04
0.11130000E+04	0.73252426E-04
0.11311000E+04	0.73620693E-04
0.11500000E+04	0.73790448E-04
0.11684000E+04	0.74816933E-04
0.11872000E+04	0.76032607E-04
0.12055000E+04	0.76736142E-04
0.12240000E+04	0.77446195E-04
0.12431000E+04	0.77603605E-04
0.12611000E+04	0.77803605E-04
0.12797000E+04	0.77983001E-04
0.12987000E+04	0.78342964E-04
0.13175000E+04	0.78704514E-04
0.13357000E+04	0.79432652E-04
0.13537000E+04	0.79983350E-04
0.13724000E+04	0.80167762E-04
0.13913000E+04	0.80723534E-04
0.14096000E+04	0.81096070E-04
0.14283000E+04	0.81470396E-04
0.14460000E+04	0.79799436E-04
0.14654000E+04	0.80352627E-04
0.14840000E+04	0.81470396E-04
0.15023000E+04	0.82224258E-04
0.15210000E+04	0.83368141E-04
0.15400000E+04	0.84139559E-04
0.15586000E+04	0.83945917E-04
0.15770000E+04	0.84139559E-04
0.15956000E+04	0.84333486E-04
0.16130000E+04	0.84527656E-04
0.16323000E+04	0.84722757E-04
0.16511000E+04	0.85310086E-04
0.16689000E+04	0.85901323E-04
0.16873000E+04	0.85113752E-04
0.17069000E+04	0.84918029E-04
0.17253000E+04	0.87096356E-04
0.17441000E+04	0.86099390E-04
0.17629000E+04	0.86297534E-04
0.17808000E+04	0.85901323E-04
0.17999000E+04	0.86296078E-04
0.18182000E+04	0.86696178E-04
0.18369000E+04	0.86896078E-04
0.18552000E+04	0.88104869E-04
0.18730000E+04	0.89125060E-04
0.18918000E+04	0.89330570E-04
0.19102000E+04	0.89125060E-04
0.19288000E+04	0.88104869E-04
0.19480000E+04	0.87096356E-04
0.19663000E+04	0.85901323E-04

Table B-10

Data for Mustard Hydrolysis at 298 K
and 0.075 Mole Fraction Ethancl

Time (sec)	$[H^+]$ (M)
0.20209999E+02	0.59156140E-07
0.38610001E+02	0.61094170E-07
0.57200001E+02	0.60394839E-07
0.75629997E+02	0.60953681E-07
0.94220001E+02	0.62661367E-07
0.11261000E+03	0.65162794E-07
0.13112000E+03	0.68548600E-07
0.14961000E+03	0.83752909E-07
0.16521001E+03	0.16143596E-06
0.18662000E+03	0.25703952E-06
0.20517999E+03	0.34673690E-06
0.22389999E+03	0.49203949E-06
0.24278000E+03	0.71614340E-06
0.26129001E+03	0.10256520E-05
0.27979001E+03	0.14927950E-05
0.29832999E+03	0.21978597E-05
0.31679001E+03	0.32433970E-05
0.33532999E+03	0.45394149E-05
0.35385999E+03	0.59566232E-05
0.37229001E+03	0.76207380E-05
0.39078000E+03	0.92632959E-05
0.40929001E+03	0.11194308E-04
0.42776000E+03	0.12971795E-04
0.44629001E+03	0.14791089E-04
0.46526001E+03	0.16443722E-04
0.48414999E+03	0.18749935E-04
0.50266000E+03	0.19769686E-04
0.52115002E+03	0.23067456E-04
0.53965997E+03	0.23983327E-04
0.55815002E+03	0.25351272E-04
0.57665997E+03	0.27164402E-04
0.59512000E+03	0.27797107E-04
0.61365997E+03	0.30060763E-04
0.63216998E+03	0.31841955E-04
0.65062000E+03	0.33189430E-04
0.66916998E+03	0.33984433E-04
0.68762000E+03	0.35237092E-04
0.70646997E+03	0.35597738E-04
0.72512000E+03	0.38725739E-04
0.74366998E+03	0.39902476E-04
0.76215002E+03	0.41086917E-04
0.78064001E+03	0.42169657E-04
0.79915002E+03	0.43651569E-04
0.81759003E+03	0.43653102E-04
0.83615002E+03	0.44666370E-04
0.85469000E+03	0.46451521E-04
0.87309003E+03	0.47206297E-04
0.89165002E+03	0.48640683E-04
0.91009003E+03	0.49431026E-04
0.92864001E+03	0.51166212E-04
0.94717999E+03	0.51760704E-04
0.96596997E+03	0.52844495E-04
0.98473003E+03	0.55082504E-04
0.10036000E+04	0.55590423E-04
0.10216000E+04	0.57147249E-04
0.10406000E+04	0.56754454E-04
0.10590000E+04	0.57544014E-04
0.10779000E+04	0.59292517E-04
0.10960000E+04	0.56210277E-04
0.11144000E+04	0.59703554E-04
0.11330000E+04	0.59156115E-04
0.11515000E+04	0.61517676E-04
0.11702000E+04	0.62230065E-04
0.11885000E+04	0.63241219E-04
0.12073000E+04	0.63386979E-04
0.12264000E+04	0.63626357E-04
0.12444000E+04	0.64365400E-04
0.12632000E+04	0.65313035E-04
0.12817000E+04	0.65463517E-04
0.12996000E+04	0.65917367E-04
0.13183000E+04	0.66527311E-04
0.13366000E+04	0.67764115E-04
0.13553000E+04	0.68233860E-04
0.13740000E+04	0.68565193E-04
0.13927000E+04	0.68591149E-04
0.14111000E+04	0.68865193E-04
0.14293000E+04	0.68706831E-04
0.14480000E+04	0.69502406E-04
0.14663000E+04	0.70307266E-04
0.14353000E+04	0.71121372E-04
0.15038000E+04	0.71779403E-04
0.15224000E+04	0.73620693E-04
0.15409000E+04	0.73960524E-04
0.15595000E+04	0.74473239E-04
0.15777000E+04	0.74989446E-04
0.15969000E+04	0.75335513E-04
0.16150000E+04	0.75683332E-04
0.16339000E+04	0.76207922E-04
0.16522000E+04	0.76913073E-04
0.16709000E+04	0.77268029E-04
0.16894000E+04	0.77624696E-04
0.17082000E+04	0.77803605E-04
0.17268000E+04	0.78162311E-04
0.17454000E+04	0.78523532E-04
0.17638000E+04	0.78704514E-04
0.17823000E+04	0.79067810E-04
0.18009000E+04	0.79432352E-04
0.18194000E+04	0.81096070E-04
0.18378000E+04	0.80723534E-04
0.18560000E+04	0.81470396E-04
0.18754000E+04	0.80909557E-04
0.18936000E+04	0.79799436E-04
0.19118000E+04	0.79250123E-04
0.19311000E+04	0.79799436E-04
0.19501000E+04	0.79067510E-04
0.19686000E+04	0.79432452E-04

Table B-11

Data for Mustard Hydrolysis at 298 K in 5% Acetone

Time (sec)	$[H^+]$ (M)
0.31700001E+02	0.45919802E-06
0.64379997E+02	0.12912186E-05
0.97050003E+02	0.37583720E-05
0.12972000E+03	0.77803643E-05
0.16239000E+03	0.11885018E-04
0.19506000E+03	0.16255479E-04
0.22773000E+03	0.21232443E-04
0.26039999E+03	0.25941796E-04
0.29307999E+03	0.29241535E-04
0.32575000E+03	0.33419510E-04
0.35842001E+03	0.39084072E-04
0.39110001E+03	0.42364267E-04
0.42410001E+03	0.44463090E-04
0.45678000E+03	0.47643101E-04
0.48945001E+03	0.53333530E-04
0.52212000E+03	0.57147849E-04
0.55479999E+03	0.58748963E-04
0.58746997E+03	0.60813498E-04
0.62014001E+03	0.64863430E-04
0.65281000E+03	0.69502406E-04
0.68548999E+03	0.71285293E-04
0.71815997E+03	0.70794522E-04
0.75084003E+03	0.73451403E-04
0.78351001E+03	0.78342964E-04
0.81619000E+03	0.79067810E-04
0.84903998E+03	0.78704514E-04
0.88171002E+03	0.79983358E-04
0.91439001E+03	0.84722757E-04
0.94707001E+03	0.86696178E-04
0.97973999E+03	0.85703788E-04
0.10124000E+04	0.85310086E-04
0.10451000E+04	0.89125060E-04
0.10778000E+04	0.91201109E-04
0.11105000E+04	0.89742905E-04
0.11431000E+04	0.88104869E-04
0.11758000E+04	0.91622001E-04
0.12085000E+04	0.94841926E-04
0.12412000E+04	0.94186974E-04
0.12740000E+04	0.92257156E-04
0.13067000E+04	0.92469789E-04
0.13394000E+04	0.94623654E-04
0.13720000E+04	0.97723649E-04
0.14047000E+04	0.99540521E-04
0.14374000E+04	0.98627897E-04
0.14701000E+04	0.95940035E-04
0.15027000E+04	0.95719421E-04
0.15354000E+04	0.95719421E-04
0.15681000E+04	0.97274729E-04
0.16008000E+04	0.97050950E-04
0.16335000E+04	0.98174831E-04
0.16662000E+04	0.98401106E-04
0.16988000E+04	0.99311619E-04
0.17317000E+04	0.99770034E-04
0.17644000E+04	0.99770034E-04
0.17971000E+04	0.99540521E-04
0.18297000E+04	0.99083161E-04
0.18624000E+04	0.99083161E-04
0.18951000E+04	0.99083161E-04
0.19278000E+04	0.98401106E-04
0.19605000E+04	0.98401106E-04
0.19932000E+04	0.97498931E-04

Time (sec)	$[H^+]$ (M)
0.20253000E+04	0.98174831E-04
0.20585000E+04	0.97949072E-04
0.20912000E+04	0.98627397E-04
0.21238999E+04	0.10069313E-03
0.21568000E+04	0.10209395E-03
0.21893999E+04	0.10327612E-03
0.22221001E+04	0.10351425E-03
0.22548000E+04	0.10375283E-03
0.22875000E+04	0.10139116E-03
0.23202000E+04	0.10046158E-03
0.23528999E+04	0.99770034E-04
0.23855000E+04	0.99770034E-04
0.24182000E+04	0.10023047E-03
0.24508999E+04	0.10162485E-03
0.24836001E+04	0.10327612E-03
0.25163000E+04	0.10471287E-03
0.25490000E+04	0.10423175E-03
0.25817000E+04	0.10423175E-03
0.26143000E+04	0.10423175E-03
0.26470000E+04	0.10399197E-03
0.26797000E+04	0.10280160E-03
0.27123999E+04	0.10280160E-03
0.27451001E+04	0.10139116E-03
0.27778000E+04	0.10232925E-03
0.28105000E+04	0.10115792E-03
0.28431001E+04	0.10092530E-03
0.28758000E+04	0.10046158E-03
0.29085000E+04	0.10046158E-03
0.29412000E+04	0.99770034E-04
0.29738999E+04	0.10046158E-03
0.30066001E+04	0.99999990E-04
0.30393000E+04	0.99311619E-04
0.30718999E+04	0.99083161E-04
0.31046001E+04	0.99770034E-04
0.31373000E+04	0.99999990E-04
0.31700000E+04	0.99770034E-04
0.32027000E+04	0.98855315E-04
0.32353999E+04	0.98627897E-04
0.32680000E+04	0.99083161E-04
0.33007000E+04	0.99540521E-04
0.33333999E+04	0.99770034E-04
0.33661001E+04	0.99999990E-04
0.33988000E+04	0.99540521E-04
0.34315000E+04	0.10023047E-03
0.34641001E+04	0.10046158E-03
0.34968000E+04	0.10069313E-03
0.35295000E+04	0.10115792E-03
0.35622000E+04	0.10069313E-03
0.35948999E+04	0.10185908E-03
0.36276001E+04	0.10209395E-03
0.36603000E+04	0.10256520E-03
0.36930000E+04	0.10280160E-03
0.37256001E+04	0.10351425E-03
0.37583000E+04	0.10303863E-03
0.37910000E+04	0.10351425E-03
0.38237000E+04	0.10399197E-03
0.38566001E+04	0.10399197E-03
0.38892000E+04	0.10375283E-03
0.39218999E+04	0.10447198E-03
0.39546001E+04	0.10375283E-03
0.39873000E+04	0.10327612E-03

Table B-11 (concluded)

Time (sec)	$[H^+]$ (M)
0.40200000E+04	0.10280160E-03
0.40527000E+04	0.10351425E-03
0.40853999E+04	0.10232925E-03
0.41181001E+04	0.10327612E-03
0.41507002E+04	0.10256520E-03
0.41833999E+04	0.10327612E-03
0.42161001E+04	0.10280160E-03
0.42487998E+04	0.10375283E-03
0.42817002E+04	0.10327612E-03
0.43142998E+04	0.10115792E-03
0.43470000E+04	0.10209395E-03
0.43797002E+04	0.10069313E-03
0.44123999E+04	0.10162485E-03
0.44451001E+04	0.10069313E-03
0.44777998E+04	0.10023047E-03
0.45103999E+04	0.10069313E-03
0.45431001E+04	0.10069313E-03
0.45757998E+04	0.10023047E-03
0.46085000E+04	0.10023047E-03
0.46412002E+04	0.10046158E-03
0.46738999E+04	0.10046158E-03
0.47066001E+04	0.99770034E-04
0.47392998E+04	0.10069313E-03
0.47718999E+04	0.10023047E-03
0.48046001E+04	0.10046158E-03
0.48372998E+04	0.10115792E-03
0.48700000E+04	0.10209395E-03
0.49027002E+04	0.10280160E-03
0.49353999E+04	0.10303863E-03
0.49681001E+04	0.10351425E-03
0.50007998E+04	0.10495422E-03
0.50333999E+04	0.10471287E-03
0.50661001E+04	0.10471287E-03
0.50987998E+04	0.10543867E-03
0.51315000E+04	0.10399197E-03
0.51642002E+04	0.10471287E-03
0.51968999E+04	0.10568169E-03
0.52296001E+04	0.10543867E-03
0.52622002E+04	0.10543867E-03
0.52948999E+04	0.10495422E-03
0.53276001E+04	0.10423175E-03
0.53602998E+04	0.10303863E-03
0.53930000E+04	0.10351425E-03
0.54257002E+04	0.10280160E-03

Table B-12

Data for Mustard Hydrolysis at 298 K
at Twice the Initial Mustard Concentration

Time (sec)	$[H^+]$ (M)
0.31700001E+02	0.16749417E-05
0.64379997E+02	0.70957726E-05
0.97050003E+02	0.15595515E-04
0.12973000E+03	0.24660409E-04
0.16239999E+03	0.32284930E-04
0.19505000E+03	0.42072646E-04
0.22775999E+03	0.50234263E-04
0.26044000E+03	0.56493689E-04
0.29310999E+03	0.66374334E-04
0.32579001E+03	0.73451403E-04
0.35847000E+03	0.78342964E-04
0.39114999E+03	0.87700057E-04
0.42400000E+03	0.95060517E-04
0.45667001E+03	0.97274729E-04
0.48935001E+03	0.10665958E-03
0.52203003E+03	0.11220186E-03
0.55470001E+03	0.11402499E-03
0.58738000E+03	0.12274394E-03
0.62004999E+03	0.12560296E-03
0.65272998E+03	0.12823303E-03
0.68540997E+03	0.13772085E-03
0.71809003E+03	0.14060468E-03
0.75076001E+03	0.14125363E-03
0.78344000E+03	0.14859356E-03
0.81612000E+03	0.15170504E-03
0.34896997E+03	0.15100800E-03
0.88165002E+03	0.15848929E-03
0.91433002E+03	0.16255488E-03
0.94700000E+03	0.15958799E-03
0.97967999E+03	0.16330522E-03
0.10124000E+04	0.16982431E-03
0.10450000E+04	0.16904403E-03
0.10777000E+04	0.16634121E-03
0.11104000E+04	0.17458230E-03
0.11431000E+04	0.17906053E-03
0.11757000E+04	0.17458230E-03
0.12084000E+04	0.17498467E-03
0.12411000E+04	0.18238943E-03
0.12738000E+04	0.18030184E-03
0.13064000E+04	0.17701088E-03
0.13391000E+04	0.18492679E-03
0.13718000E+04	0.18535301E-03
0.14045000E+04	0.17988707E-03
0.14371000E+04	0.18492679E-03
0.14698000E+04	0.18967057E-03
0.15025000E+04	0.18492679E-03
0.15352000E+04	0.18535301E-03
0.15678000E+04	0.19275244E-03
0.16005000E+04	0.19010789E-03
0.16332000E+04	0.18578040E-03
0.16659000E+04	0.19364218E-03
0.16985000E+04	0.19142560E-03
0.17314000E+04	0.18879908E-03
0.17640000E+04	0.19769697E-03
0.17967000E+04	0.19186681E-03
0.18294000E+04	0.19230903E-03
0.18621000E+04	0.19998614E-03
0.18947000E+04	0.19319659E-03
0.19274000E+04	0.19498439E-03
0.19601000E+04	0.20183665E-03
0.19928000E+04	0.19543379E-03
0.20254000E+04	0.19769697E-03
0.20581001E+04	0.20276831E-03
0.20908000E+04	0.19633608E-03
0.21235000E+04	0.19633608E-03
0.21563000E+04	0.20276831E-03
0.21890000E+04	0.20230185E-03
0.22217000E+04	0.19588441E-03
0.22543000E+04	0.19998614E-03
0.22870000E+04	0.20276831E-03
0.23197000E+04	0.19543379E-03
0.23523999E+04	0.19724235E-03
0.23850000E+04	0.20464454E-03
0.24177000E+04	0.19724235E-03
0.24503999E+04	0.19498439E-03
0.24831001E+04	0.20137233E-03
0.25157000E+04	0.19860952E-03
0.25483999E+04	0.19230903E-03
0.25812000E+04	0.19769697E-03
0.26138999E+04	0.20183665E-03
0.26466001E+04	0.19453601E-03
0.26793000E+04	0.19453601E-03
0.27120000E+04	0.20090927E-03
0.27446001E+04	0.19815261E-03
0.27773000E+04	0.19364218E-03
0.28100000E+04	0.19633608E-03
0.28427000E+04	0.20090927E-03
0.28753000E+04	0.19364218E-03
0.29080000E+04	0.19633608E-03
0.29407000E+04	0.20090927E-03
0.29733999E+04	0.19275244E-03
0.30062000E+04	0.19498439E-03
0.30388999E+04	0.20183665E-03
0.30715000E+04	0.19498439E-03
0.31042000E+04	0.19498439E-03
0.31368999E+04	0.20044728E-03
0.31696001E+04	0.19588441E-03
0.32022000E+04	0.19408867E-03
0.32348999E+04	0.20137233E-03
0.32676001E+04	0.19678861E-03
0.33003000E+04	0.19453601E-03
0.33328999E+04	0.19998614E-03
0.33656001E+04	0.19186681E-03
0.33983000E+04	0.19906728E-03
0.34311001E+04	0.19543379E-03
0.34638000E+04	0.19588441E-03
0.34965000E+04	0.19952627E-03
0.35291001E+04	0.19230903E-03
0.35618000E+04	0.19906728E-03
0.35945000E+04	0.19230903E-03
0.36272000E+04	0.19860952E-03
0.36598000E+04	0.19364218E-03
0.36925000E+04	0.19633608E-03
0.37252000E+04	0.19678861E-03
0.37578999E+04	0.19319639E-03
0.37906001E+04	0.19952627E-03
0.38232000E+04	0.19098523E-03
0.38561001E+04	0.19998614E-03
0.38887000E+04	0.19098523E-03
0.39213999E+04	0.19815261E-03
0.39541001E+04	0.19453601E-03
0.39868000E+04	0.19588441E-03

Table B-12 (concluded)

Time (sec)	$[H^+]$ (M)
0.40193999E+04	0.19678861E-03
0.40521001E+04	0.19275244E-03
0.40848000E+04	0.19860952E-03
0.41175000E+04	0.19186681E-03
0.41501001E+04	0.19952627E-03
0.41827998E+04	0.19142560E-03
0.42155000E+04	0.19952627E-03
0.42482002E+04	0.19054607E-03
0.42810000E+04	0.19815261E-03
0.43137002E+04	0.19275244E-03
0.43463999E+04	0.19815261E-03
0.43790000E+04	0.19319689E-03
0.44117002E+04	0.19906728E-03
0.44443999E+04	0.19098523E-03
0.44771001E+04	0.19998614E-03
0.45097002E+04	0.19186681E-03
0.45423999E+04	0.20090927E-03
0.45751001E+04	0.19186681E-03
0.46077998E+04	0.20044728E-03
0.46405000E+04	0.19142560E-03
0.46731001E+04	0.19906728E-03
0.47057998E+04	0.19098523E-03
0.47385000E+04	0.19860952E-03
0.47712002E+04	0.19364218E-03
0.48037998E+04	0.19633608E-03
0.48365000E+04	0.19408867E-03
0.48692002E+04	0.19453601E-03
0.49018999E+04	0.19588441E-03
0.49345000E+04	0.19230903E-03

Table B-13

The Data for Hydrolysis of Chloroethyl Ethyl Sulfide in 5% Acetone/Water (V/V) at 298 K

.ime (sec)	$[H^+]$ (M)
0.82299995E+01	0.11508001E-06
0.15230000E+02	0.63386942E-05
0.22240000E+02	0.29853813E-04
0.29250000E+02	0.42364267E-04
0.36250000E+02	0.49888415E-04
0.43259998E+02	0.58884369E-04
0.50259998E+02	0.66680645E-04
0.57270000E+02	0.72777977E-04
0.64279999E+02	0.78523532E-04
0.71279999E+02	0.84139559E-04
0.78290001E+02	0.86099390E-04
0.85370003E+02	0.91201139E-04
0.92629997E+02	0.93325332E-04
0.99639999E+02	0.95940035E-04
0.10664000E+03	0.99083161E-04
0.11365000E+03	0.10162485E-03
0.12065000E+03	0.10069313E-03
0.12766000E+03	0.10280160E-03
0.13467000E+03	0.10447198E-03
0.14167000E+03	0.10495422E-03
0.14867999E+03	0.10568169E-03
0.15567999E+03	0.10214340E-03
0.16269000E+03	0.10616951E-03
0.16969000E+03	0.10939562E-03
0.17687000E+03	0.10814340E-03
0.18420000E+03	0.10789462E-03
0.19121001E+03	0.11015389E-03
0.19821001E+03	0.11117315E-03
0.20522000E+03	0.11091751E-03
0.21222000E+03	0.11066235E-03
0.21923000E+03	0.10889299E-03
0.22623000E+03	0.10964776E-03
0.23324001E+03	0.11040788E-03
0.24024001E+03	0.11168632E-03
0.24725000E+03	0.10990058E-03
0.25425999E+03	0.11142939E-03
0.26126001E+03	0.11350105E-03
0.26856000E+03	0.11246046E-03
0.27594000E+03	0.11194374E-03
0.28294000E+03	0.11040788E-03
0.28995001E+03	0.11040738E-03
0.29695001E+03	0.11066235E-03
0.30395999E+03	0.11194374E-03
0.31095999E+03	0.10990058E-03
0.31797000E+03	0.11246046E-03
0.32498001E+03	0.11246046E-03
0.33198001E+03	0.11168632E-03
0.33898999E+03	0.10939562E-03
0.34598999E+03	0.10964776E-03
0.35300000E+03	0.10939562E-03
0.36025000E+03	0.11040788E-03
0.36751001E+03	0.11066235E-03
0.37451001E+03	0.11015389E-03
0.38151999E+03	0.10964776E-03
0.38851999E+03	0.11091751E-03
0.39551999E+03	0.10914406E-03
0.40253000E+03	0.10839265E-03
0.40954001E+03	0.11117315E-03
0.41654001E+03	0.11117315E-03
0.42354999E+03	0.10864258E-03
0.43054999E+03	0.11040788E-03

Time (sec)	$[H^+]$ (M)
0.43756000E+03	0.11040788E-03
0.44456000E+03	0.11066235E-03
0.45157001E+03	0.11040788E-03
0.45879001E+03	0.11091751E-03
0.46607999E+03	0.10964776E-03
0.47307999E+03	0.10964776E-03
0.48009000E+03	0.10939562E-03
0.48710001E+03	0.10739853E-03
0.49410001E+03	0.10939562E-03
0.50110999E+03	0.11040788E-03
0.50810999E+03	0.10990058E-03
0.51512000E+03	0.10914406E-03
0.52212000E+03	0.11040788E-03
0.52913000E+03	0.11015389E-03
0.53614001E+03	0.10939562E-03
0.54314001E+03	0.10939562E-03
0.55032001E+03	0.11040788E-03
0.55765002E+03	0.11040788E-03
0.56465997E+03	0.10939562E-03
0.57165997E+03	0.10964776E-03
0.57866998E+03	0.10990058E-03
0.58567999E+03	0.10889299E-03
0.59267999E+03	0.10914406E-03
0.59969000E+03	0.10964776E-03
0.60669000E+03	0.10764651E-03
0.61370001E+03	0.11015389E-03
0.62071002E+03	0.11040788E-03
0.62771002E+03	0.109395[illegible]E-03
0.63471997E+03	0.10814340E-03
0.64202002E+03	0.10914406E-03
0.64922998E+03	0.10914406E-03
0.65622998E+03	0.10939562F-03
0.66323999E+03	0.11015389E-03
0.67025000E+03	0.11066235E-03
0.67725000E+03	0.10964776E-03
0.68426001E+03	0.11040788E-03
0.69126001E+03	0.10964776E-03
0.69827002E+03	0.10839265E-03
0.70527002E+03	0.10864258E-03
0.71228003E+03	0.10914406E-03
0.71928003E+03	0.11015389E-03
0.72623998E+03	0.10990058E-03
0.73353998E+03	0.10964776E-03
0.74079999E+03	0.10914406E-03
0.74779999E+03	0.10889299E-03
0.75481000E+03	0.11015339E-03
0.76182001E+03	0.10990058E-03
0.76882001E+03	0.10990058E-03
0.77583002E+03	0.11117315E-03
0.78284003E+03	0.11015389E-03
0.78984003E+03	0.10964776E-03
0.79684998E+03	0.10939562E-03
0.80384998E+03	0.11066235E-03
0.81085999E+03	0.11015389E-03
0.81785999E+03	0.10964776E-03
0.82508002E+03	0.10 [illegible]4776E-03
0.83237000E+03	0.11015389E-03
0.83938000E+03	0.11015389E-03
0.84639001E+03	0.11066235E-03
[illegible]	0 [illegible]08392 65E-03
[illegible]	[illegible]964776[illegible] 03
0.86740997E+03	0.10964776E-03
0.87440997E+03	0.10990058E-03
0.88141998E+03	0.10964776E-03
0.88841998E+03	0.10814340E-03

Appendix C

pH STAT CONTROL PROGRAM USER'S GUIDE

I. Introduction

The pHstat program monitors the acidity of up to four reactions and adds titrant as needed to maintain pH at a user selected setpoint. It is written in the BASIC language and runs on a DEC MINC computer in BASIC mode. The program has the ability to set initial pH before the user initiates the reaction, add titrant (either according to a "speed factor" or a stoichiometric method), record pH and cumulative pH as a function of time, and write results to a file that can then be analyzed by other programs. Program flow is controlled by means of selections from a specified menu.

II. Setting up to run the program

To run the program, it is necessary to connect lines from each pH meter to the computer and also a line from the computer to the pH stat controller box. To connect the lines from the pH meters to the MINC, find the four A/D channels in front of the computer. These are labelled 0,1,2 and 3, corresponding to meters 1,2,3, and 4. If less than four stats are being used, they should be connected so that the lower numbered A/D channels are used (that is, if only three stats are being used, connect them to channels, 0,1, and 2). To connect a line to a channel, line up the pins on the channel terminal with the slots in the sleeve of the line connector, push the connector over the terminal, and rotate the sleeve about a quarter of a turn clockwise. You should be able to feel the connector lock. The line from the computer labelled "controller" (if the label is gone, it is the line with the round multi-pin connector) should be connected to the back of the pHstat controller. Simply line up the notch in the receptacle with the tab in the connector and push (it can only go in the right way).

To "boot up" the BASIC system, insert a copy of the system disk containing the PHSYS program, into the leftmost disk drive on the MINC and turn on the power switch (the red switch a little right of center

on the front of the computer). If save data files are to be written, an initialized data disk may be inserted into the rightmost drive at this time (or for that matter, at any time before you are ready to control a reaction's pH).

After several seconds, the system prompts for the date. The expected format is DD-MMM-YY, where DD is the day (numeric), MMM is the 3-character abbreviation of the name of the month, and YY is the year. An example of a valid date string is "9-MAR-84." Note that you do not need to insert a leading zero before the day to get it to two digits. The next prompt given by the system is for clock time, and you should answer in the form HH:MM:SS for hours, minutes, and seconds. Hours should be given in 24-hour clock time, and seconds may be omitted. After a few seconds the message READY is displayed on the screen. You may run the PHSYS program at this point by typing RUN PHSYS. The computer responds by displaying the PHSYS menu on the terminal screen.

1. Enter or change parameters
2. Calibrate pH meters
3. Enter or change setpoints
4. Set initial pH
5. Control reaction pH
6. Exit program

The numeric order of the menu items is approximately the order in which they would be selected in a typical run, although the actual order can be flexible and the program has a lot of internal default values. All menu items other than the sixth can be selected more than once in a given run. To select a menu item, simply type the corresponding number through the terminal keyboard. Each item is discussed in more detail below.

1. Enter or change parameters

This item allows the user to set or reset the run parameters. Parameters that may be set are the number of stats, the number of

readings to average for each pH reading, whether speed factor or stoichiometric titration is to be done, and the pH meter factors A and B. For all parameter input, if the program has an initial or current value, that value is kept unchanged if you hit return in response to the prompt. For reference purposes, the initial or current value is printed. The exact meaning of each of these parameters is as follows:

Number of stats : Answer with the number of stats, if different from the current value (which is printed for reference). Must be numeric between 1 and 4. Initial defaul value is 4.

Number of seconds between each reading : Answer with the number of seconds between each reading of the pH meters. The value must be between .1 and 600 seconds. The initial value is .1 seconds.

Number or readings to average for each pH : This number of readings are averaged to come up with a pH value that is written to the screen while pH is being controlled. Combined with the number or seconds between readings, the user can control the rate at which titrant is added and also the number of points written to the save data files (if any). For example, if the user wishes to add titrant not more than once every 10 seconds, a possible combination of values for these two parameters would be one second between readings and ten readings to be averaged. If the experiment runs for 15 minutes, 90 points (900 seconds divided by 10 seconds/point) will be written to the save files. As a general guideline, the number of seconds between readings multiplied by the number of readings to average for each pH should be small relative to the reaction's expected or approximate half-life. By default, 25 readings will be averaged for each pH. These two parameters do not affect the rate of titration when menu item 4 (Set initial pH) is selected; in that case, the MINC adjusts the pH as quickly as it can.

Speed factor versus stoichiometric control : speed factor titration is selected by typing 1 in response to the prompt "Enter 1 for speed factor or 2 for stoichiometric control," while typing

2 results in stoichiometric control. If speed factor control is chosen, the next prompt is for the speed factor itself. The meaning of the speed factor is that PHSYS will add that number of squirts (each 2.5 microliter) of titrant for each pH unit that the solution in question is off from the setpoint. For example, if speed factor is 20, pH is 6.5, and setpoint pH is 7, PHSYS will add (7-6.5)*20 or 10 squirts to the solution. If stoichiometric control is requested, the program prompts for the initial reaction volume in liters and an overshoot factor. In this mode, the program computes the amount of titrant to be added stoichiometrically (based on the reaction pH and the normal concentration of the titrant) and then increases this amount according to the overshoot factor. A factor of 5, for example, tells the program to compute the amount of titrant to add and then to increase this amount by 5%. A small overshoot factor is desirable if pH is tending steadily away from the set point between titrant additions because then the average of the readings between additions will be biased towards the set point and the computed amount of titrant will be insufficient to bring the reaction back to the set point.

pH meter factors A and B : The default values of A and B are .942 and 7, respectively. The user will not generally need to change these as long as he or she is using the standard "blue box" between the pH electrodes and the MINC. The program computes pH from a voltage signal from the blue box by multiplying the voltage by A and adding B. For example, a voltage of 0 corresponds to pH 7 (0*A + B = 7) while a voltage of -1 corresponds to pH 6.057 (-1*A + B).

2. Calibrate pH meters

For reactions tending towards acidic pH, the meters should be calibrated at pH 4 and 7. Otherwise, the meters should be calibrated at pH 10 and 7. All reactions for a given run of PHSYS should be tending in the same direction. For best calibration results, the pH meters should be allowed some time to warm up (a figure of 30 minutes is given in the design article, but at least a few minutes would be better than nothing).

The first prompt from PHSYS in the calibration procedure asks the user whether the reaction is going acidic or basic. Enter A for reactions going acidic, B for those going basic. The user is then told to place the electrodes in a pH 7 buffer and adjust the CAL knob until a pH reading of 7 appears on the terminal screen (one CAL knob per stat). After pH 7 is obtained, the user hits any key (for example, <return>) to continue. The instructions on the screen then tell the user to place the electrodes in a pH 4 (for acid-tending) or 10 (for basic-tending) buffer and adjust SLOPE until the desired value is obtained. Again, the user presses any key when done. At this point, the user may type "R" to repeat the calibration procedure or <return> to return to the main menu.

3. Enter or change setpoints

This menu item is selected to establish set point pH values for each stat, that is, those pH values at which the PHSYS program will try to maintain each reaction. Note that each stat may have a different set point. If no set points had previously been defined, the program prompts the user for the setpoint value for each stat (there is no initial default value for set point pH). After values have been entered, the user is given the opportunity to change one or more of them by entering the appropriate stat number and then the new value. Hitting <return> for stat number brings about a return to the main menu, while hitting <return> for the value prompt retains the current value (which is printed for the user's information) but leaves the user in the set point change procedure. If the user tries to set initial pH or control reaction pH (menu items 4 or 5) without having given set point values, the PHSYS program automatically invokes the set point procedure before continuing.

4. Set initial pH

This menu item is used to bring the solvent pH to the set point value before the reaction is initiated. If no set points have been given, the program invokes that procedure before setting initial pH.

The first prompt is for acidic or basic titrant. The user should enter 1 for acid or -1 for basic (the titrants for all the stats must be either acidic or basic). If stoichiometric adjustment had been requested in the parameter section, the program prompts for titrant concentration in normal units for each stat. Different normal concentrations for the titrant in each stat are allowed. The user is then prompted for the percent tolerance within which solvent pH should be adjusted to set point pH. Adjustment will continue until solvent pH is within this percent tolerance for each stat. The default value is 1 %. Therefore, for example, if pH 7 is the setpoint for a particular stat, adjustment will continue until pH in that stat is between 6.93 and 7.07, that is, 7 plus or minus one per cent. At this point, the program gives the various concentration and tolerance and allows the user to correct them if needed. Entering 'C' allows the user to correct these values, while hitting <return> starts the procedure. As usual, hitting <return> for a prompt for a value already known to the program causes that value to be retained.

Two problems could throw this procedure into a very long or even infinite loop. The first is the selection of an excessively tight tolerance, so that the program can never bring all the stats within the acceptable limits. The second is that since titrant of only one type (acidic or basic) is being added, if the solvent goes too far on the other side of the set point it will never be within the desired per cent tolerance. Fortunately, the initial pH adjustment procedure can be terminated by hitting the character 'X' (without a <return> while the procedure is running. The message "initial adjustment stopped by user" is printed, and you can get back to the main menu by hitting <return>. If all stats are successfully adjusted within the desired per cent tolerance, the message "All stats are within x % of setpts" is printe and again you can get back to the main menu by hitting <return>. You may, if you wish, re-enter this procedure by selecting menu item 4 again. An example of when you may want to do this is when the program fails to adjust initial pH and you stop it, and then replace the solvents with more stable ones or are willing to accept a larger tolerance.

5. Control reaction pH

Usually, you would enter this menu item before you start the reaction. After everything is set up, you will have a pause during which you can start your reaction and hit <return>, enabling you to get a reasonably accurate start time.

As with menu item 4, if no set point pH values have been given, the set point procedure is invoked before continuing. The next prompt, again as in menu item 4, is to enter 1 for acidic titrant or -1 for basic (this prompt is bypassed if item 4 had been previously selected). If stoichiometric adjustment is in effect, the next prompt is for normal concentration of titrant in each stat (again, this is bypassed if these values had been entered under item 4). Following these, the program asks for the time limit for the experiment in minutes. The program will add titrant as needed and collect data up to this time limit. Next you are asked for the file name to which to write the data for further analysis. The name you enter should not contain extensions (that is, things like .dat). You may hit <return> if you do not want a data file from this experiment. The name that you enter is truncated to 5 characters and the volume and type extensions are appended by the program automatically. Though you only enter one name, the program will create as many files as there are stats. All data files are written to drive SY1:, so be sure you have a disk there before answering this prompt or a fatal error will result. As an example of file name generation, suppose you entered "SCRATCH" in response to file name and there are 3 stats. The program would then proceed to open files SY1:SCRAT1.DAT, SY1:SCRAT2.DAT, and SY1:SCRAT3.DAT. These files may be examined on the screen by entering "TYPE SY1:SCRAT1.DAT" in response to the READY prompt (to type the first one) and may be transfered to the VAX.

The program now displays all this information and gives you a chance to correct it by typing "C" followed by <return>. If every item is correct, start your reaction and hit <return>. The reaction time clock is started when you hit this return.

As with setting initial pH, you may terminate the control run by hitting the character "X" during the control phase. If you stop the reaction by hitting "X", the message "Run terminated by user" is printed. If you let the reaction run out to the time limit, the message "Normal run termination" is printed. In either case, the files created (if any) will be properly closed, and hitting <return> get you back to the main menu.

6. Exit program

Enter this menu item to stop program execution. This is the prefered way to stop the program, as opposed to more traumatic methods such as control-C and turning the machine off. Stopping via this menu item properly closes all save files.

IV. Pertinent Equations

Voltage to pH

The blue box connected between the pH electrodes and the MINC functions as an amplifier for the electrode voltage. It sends a voltage (call it V) to the MINC for each stat. This is converted to pH by the equation

$$pH = A*V + B$$

where A and V are pH meter factors A and B (.942 and 7 for the usual blue box). Other types of amplifiers may require different values of A and B for the above equation to give the correct pH. The amplifier should be designed or adjusted so that no expected pH is converted to a voltage outside the range -5.11 to 5.12 volts, as the MINC will set these values to the endpoints of this range and the recorded pH will be incorrect.

Number of squirts (speed factor)

Let pH be actual pH, pH(S) be setpoint pH, F be the speed factor, and D be +1 for acidic or -1 for basic titrants. Then the number of squirts added to a given stat will equal

$$Y = (pH - pH(S))*D*F$$

rounded to the nearest integer. If the computed Y is less than 0, no titrant is added (so note that the adjustment can only go one way).

Number of squirts (stoichiometric)

Let pH, pH(S), and D be as above, F be the percent overshoot factor, M be the normal concentration of titrant, V1 be the current reaction volume, and V2 be the volume per squirt. Then

$$X = (10(-pH)-10(-pH(S)))*V1/(V2*M)$$

$$Y = (-D*X)*(1+F/100)$$

As under the speed factor method, Y is rounded to the nearest integer, and negative values of Y are set to 0. The new reaction volume V1 is then given by

$$V1 = V1 + V2*Y$$

```
10 REM PHSTAT S.E.JACKSON 5/83
20 REM UPDATED A VALUES 3/84
30 N2=25 \ A=.942 \ B=7 \ S=50
40 N=4
50 DIM X(3),P(3),N1(3),S2(3),V0(3),V1(3),M(3)
60 DIM D1(3),D2(3),C1(3)
70 REM
80 D9=2000
90 F9=0
100 F2=1
110 T1=.1
120 FOR I=0 TO 3
130 S2(I)=-1 \ V0(I)=0 \ V1(I)=0
140 NEXT I
150 D=0
160 M=0
170 V2=2.50000E-06
180 REM
190 REM
200 DISPLAY_CLEAR
210 PRINT 'pH Stat Controller, Version 2.0, March 1984.'
220 PRINT
230 PRINT  \ PRINT 'MAIN MENU:' \ F1=0
240 PRINT '1= Enter or change Parameters' \ PRINT '2= Calibrate pH meter
250 PRINT '3= Enter or change setpoints'
260 PRINT '4= Set initial pH'
270 PRINT '5= Control reaction pH'
280 PRINT '6= Exit program'
290 PRINT
300 PRINT 'Menu items other than 6 may be selected several times in a r
310 PRINT
320 PRINT 'Enter your choice followed by <return> :';
330 INPUT P1
340 P1=INT(P1)
350 IF P1<=0 THEN 380
360 IF P1=6 THEN STOP
370 IF P1<=5 THEN 400
380 PRINT 'Between 1 and 6 please !'
390 GO TO 320
400 ON P1 GOSUB 770,1430,3500,1670,1370
410 GO TO 200
420 REM READ Ph
430 FOR I=0 TO N-1 \ P(I)=0 \ NEXT I
440 N6=10
450 IF P1=5 THEN N6=N2
460 FOR J=1 TO N6
470 IF P1<>5 GO TO 500
480 GET_TIME(S1)
490 IF (S1-S0)<T1-.07*N THEN 480
500 AIN(,X(),N,0,0,N)
510 S0=S1
520 FOR I=0 TO N-1 \ P(I)=P(I)+X(I) \ NEXT I
530 NEXT J
540 FOR I=0 TO N-1 \ P(I)=P(I)/N6*A+B \ NEXT I
550 IF F1<>99 THEN  GOSUB 580
560 RETURN
570 REM
580 REM PRINT ON SCREEN
590 MOVE_CURSOR(1,1)
600 IF P1<>5 THEN 620
610 PRINT 'Adjusting pH. Running time (sec) : ';T3
```

```
620 PRINT
630 PRINT 'Stat  Setpt pH   Actual pH   ';
640 IF P1<>5 THEN PRINT
650 IF P1=5 THEN PRINT 'Time(sec)    Squirts    Cum squirts'
660 FOR I=0 TO N-1
670 PRINT USING '  #    #.###       #.###     ';I+1;S2(I);F(I);
680 IF P1=5 THEN 710
690 PRINT
700 GO TO 720
710 PRINT USING '#.####^^^^  #.####^^^^  #.####^^^^';D2(I);D1(I);C1(I)
720 NEXT I
730 RETURN
740 REM
750 INPUT X$ \ X1=VAL(X$)
760 RETURN
770 REM
780 REM PARAMETER ENTRY
790 DISPLAY_CLEAR
800 PRINT 'Enter new value or <RETURN> for no change.'
810 PRINT
820 PRINT 'Number of stats, now = ';N;' : ';
830 GOSUB 750
840 IF X1<=0 THEN 890
850 IF X1<=4 THEN 880
860 PRINT 'Between 1 and 4 please !'
870 GO TO 820
880 N=X1
890 REM
900 PRINT 'Seconds between readings (.1 to 600), now = ';T1
910 GOSUB 750
920 IF X1=0 THEN X1=T1
930 IF X1>=.1 THEN IF X1<=600 THEN T1=X1
940 IF X1>600 THEN 960
950 IF X1>0 THEN IF X1>=.1 THEN 980
960 PRINT 'Between .1 and 600 please !'
970 GO TO 900
980 REM
990 PRINT 'Number of readings to average for each pH, now = ';N2;' : ';
1000 GOSUB 750
1010 IF X1>=1 THEN N2=INT(X1)
1020 PRINT 'Enter 1 for speed factor or 2 for stoich. control (now ';F2;' ) ';
1030 GOSUB 750
1040 IF X1=0 GO TO 1120
1050 IF X1>0 GO TO 1080
1060 F2=1
1070 GO TO 1120
1080 IF X1<=2 GO TO 1110
1090 PRINT '1 or 2 please !'
1100 GO TO 1020
1110 F2=X1
1120 REM
1130 IF F2=2 THEN 1200
1140 REM ENTER FACTOR
1150 PRINT 'Speed factor, now ';S;' : ';
1160 GOSUB 750
1170 IF X1>0 THEN S=INT(X1)
1180 GO TO 1390
1190 REM
1200 REM STOICH METHOD-NEED VOLUME
1210 FOR I=1 TO N
1220 PRINT 'Initial solution volume (liter) for Stat ';I;' : ';
```

```
1230 IF VO(I-1)>0 THEN PRINT '(now ';VO(I-1);' ) ';
1240 GOSUB 750
1250 IF X1=0 THEN IF VO(I-1)>0 GO TO 1310
1260 IF X1>0 GO TO 1290
1270 PRINT 'Greater than 0 please !'
1280 GO TO 1220
1290 VO(I-1)=X1
1300 V1(I-1)=VO(I-1)
1310 NEXT I
1320 PRINT 'Overshoot factor (percent), now ';F9*100;' : ';
1330 GOSUB 750
1340 IF X1=0 THEN 1390
1350 IF X1>0 THEN 1380
1360 PRINT 'Greater than 0 please !'
1370 GO TO 1320
1380 F9=X1/100
1390 REM
1400 PRINT 'pH meter factor A, now ';A;' : ';
1410 GOSUB 750
1420 IF X1>0 THEN A=X1
1430 PRINT 'pH meter factor B, now ';B;' : ';
1440 GOSUB 750
1450 IF X1>0 THEN B=X1
1460 RETURN
1470 REM
1480 REM CALIBRATE
1490 DISPLAY_CLEAR
1500 MOVE_CURSOR(12,1)
1510 PRINT 'Is reaction going acidic(A) or basic(B) ';
1520 INPUT X$
1530 IF X$='a' THEN X$='A'
1540 IF X$='b' THEN X$='B'
1550 IF X$='A' GO TO 1590
1560 IF X$='B' THEN 1610
1570 PRINT 'A or B please !'
1580 GO TO 1510
1590 P9=4
1600 GO TO 1620
1610 P9=10
1620 DISPLAY_CLEAR \ MOVE_CURSOR(12,1)
1630 PRINT 'Place electrodes in pH 7 buffer. Adjust CAL until pH = 7.'
1640 PRINT 'Press any key when done. '
1650 GOSUB 420
1660 GOSUB 1830
1670 IF X$='' THEN 1650
1680 DISPLAY_CLEAR \ MOVE_CURSOR(12,1)
1690 PRINT 'Place electrodes in pH ';P9;' buffer. Adjust SLOPE until pH = ';P9
1700 PRINT 'Press any key when done.'
1710 REM
1720 GOSUB 420
1730 GOSUB 1830
1740 IF X$='' THEN 1720
1750 DISPLAY_CLEAR \ MOVE_CURSOR(12,1)
1760 PRINT 'Enter R to recalibrate or any other key to get back to main menu.'
1770 GOSUB 420
1780 GOSUB 1830
1790 IF X$='' THEN 1770
1800 IF X$='R' THEN 1480
1810 IF X$='r' THEN 1480
1820 RETURN
1830 REM
```

```
1840 GET_CHAR(X$)
1850 RETURN
1860 REM
1870 REM
1880 REM CONTROL PH
1890 DISPLAY_CLEAR
1900 MOVE_CURSOR(12,1)
1910 IF P1=5 THEN F1=99
1920 IF P1=4 THEN F1=0
1930 IF S2(0)>0 THEN 1950 \ REM ENTER SETPOINTS
1940 GOSUB 3490
1950 DISPLAY_CLEAR
1970 PRINT 'Input 1 for acid titrant, -1 for basic : ';
1980 IF D<>0 THEN PRINT '(now ';D;' ) ';
1990 GOSUB 750
2000 X1=INT(X1)
2010 IF X1<>0 THEN D=X1
2020 IF ABS(D)=1 THEN 2050
2030 PRINT '1 or -1 please !'
2040 GO TO 1960
2050 REM
2060 FOR I=0 TO N-1 \ N1(I)=0 \ D1(I)=0 \ C1(I)=0
2070 IF F2=1 THEN 2160
2080 PRINT 'Concentration (NORMAL units) of titrant, Stat # ';I+1,'  : ';
2090 IF M(I)>0 THEN PRINT '(now ';M(I);' ) ';
2100 GOSUB 750
2110 IF X1=0 THEN IF M(I)>0 THEN 2160
2120 IF X1>0 THEN 2150
2130 PRINT 'Greater than 0 please !'
2140 GO TO 2080
2150 M(I)=X1
2160 NEXT I
2170 REM TIME,FILE,ID FOR ITEM 5
2180 IF P1=4 THEN 2510
2190 PRINT 'Time limit for experiment (minutes) : ';
2200 GOSUB 750
2210 IF X1>0 THEN 2240
2220 PRINT 'Greater than 0 please !'
2230 GO TO 2190
2240 T2=60*X1
2250 PRINT 'Save file name, <RETURN> for no file : ';
2260 INPUT F$
2270 IF F$='' THEN 2330
2280 F$=SEG$(F$,1,5)
2290 FOR I=1 TO N
2300 I$='SY1:'+F$ \ I$=I$+STR$(I) \ I$=I$+'.DAT'
2310 OPEN I$ FOR OUTPUT AS FILE #I
2320 NEXT I
2330 PRINT 'Enter run ID : ';
2340 INPUT I$
2350 IF F$='' THEN 2400
2360 FOR I=1 TO N
2370 PRINT #I,I$;' STAT # ';I
2380 PRINT #I,'TIME';TAB(14);'PH';TAB(20);'SQUIRTS   CUM SQUIRTS'
2390 NEXT I
2400 DISPLAY_CLEAR
2410 GOSUB 3400
2420 MOVE_CURSOR(12,1)
2430 PRINT 'Hit <RETURN> to begin, or C to correct these ';
2440 INPUT X$
2450 IF X$='C' THEN 1890
```

```
2460 IF X$='c' THEN 1890
2470 DISPLAY_CLEAR
2480 MOVE_CURSOR(12,1)
2490 PRINT 'Controlling pH. Press X to terminate run.'
2500 GO TO 2690
2510 REM P1=4 - SET INITIAL PH
2520 DISPLAY_CLEAR \ MOVE_CURSOR(12,1)
2530 PRINT 'Setpoint tolerance(pct). Adjustment will continue till each'
2540 PRINT 'stat is within this pct tolerance of its setpoint (default 1%) :
2550 GOSUB 750
2560 IF X1=0 THEN X1=1
2570 IF X1>0 THEN 2600
2580 PRINT 'Greater than 0 please !'
2590 GO TO 2530
2600 E1=X1/100
2610 DISPLAY_CLEAR
2620 GOSUB 3400
2630 PRINT 'Hit <RETURN> to begin adjustment, C to correct these ';
2640 INPUT X$
2650 IF X$='C' GO TO 1890
2660 IF X$='c' GO TO 1890
2670 DISPLAY_CLEAR
2680 PRINT 'Adjusting initial pH. Press X to return to main menu.'
2690 START_TIME('CHZ')
2700 GET_TIME(S0) \ REM INITIAL S0-RUNNING S0 KEPT IN PH READ GOSUB
2710 REM start
2720 GOSUB 420
2730 FOR I=0 TO N-1
2740 GOSUB 3280
2750 IF Y<=0 THEN 2900
2760 IF P1=4 THEN 2830
2770 IF N1(I)=D9 THEN 3060
2780 N1(I)=N1(I)+1
2790 D1(I)=Y
2800 C1(I)=C1(I)+Y
2810 GET_TIME(T3)
2820 D2(I)=T3
2830 FOR J=1 TO Y
2840 SET_LINE(I,1)
2850 SET_LINE(I,0)
2860 NEXT J
2870 IF P1=4 THEN 2900
2875 IF F$='' THEN 2900
2880 PRINT #I+1,USING '#.####^^^^  #.###   ####',D2(I),P(I),D1(I);
2890 PRINT #I+1,USING '      ########',C1(I)
2900 NEXT I
2910 GET_TIME(T3)
2920 GOSUB 580
2930 GET_CHAR(X$) \ IF X$='X' THEN 3060
2940 IF P1=4 THEN 2970
2950 IF T3>=T2 THEN 3060
2960 GO TO 2710
2970 REM
2980 REM CHECK ERROR TOL E0
2990 E0=0
3000 FOR I=1 TO N
3010 X1=ABS(P(I-1)-S2(I-1))/P(I-1)
3020 IF X1>E0 THEN E0=X1
3030 NEXT I
3040 IF E0<=E1 GO TO 3060
3050 GO TO 2710
```

```
3060 REM END ADJ OR CONTROL-SAVE IF P1=5
3070 START_TIME('HALT')
3080 MOVE_CURSOR(15,1)
3090 IF P1=4 THEN 3190
3100 IF X$='X' THEN 3130
3110 PRINT 'Normal run termination.'
3120 GO TO 3140
3130 PRINT 'Run terminated by user.'
3140 IF F$='' THEN 3250
3150 FOR I=1 TO N
3160 CLOSE #I
3170 NEXT I
3180 GO TO 3250
3190 REM
3200 REM
3210 IF X$='X' GO TO 3240
3220 PRINT 'All stats within ';E1*100;' pct of setpts. '
3230 GO TO 3250
3240 PRINT 'Initial adjustment stopped by user. '
3250 PRINT 'Hit <RETURN> to return to main menu. ';
3260 INPUT X$
3270 RETURN
3280 REM COMPUTE NO. OF SQUIRTS Y
3290 REM F2=1 : SPEED FACTOR, 2 : STOICH
3300 IF F2=2 GO TO 3340
3310 Y=INT((P(I)-S2(I))*S*D+.5)
3320 GO TO 3370
3330 REM
3340 Y=((10^(-P(I))-10^(-S2(I)))*(V1(I)/V2))/M(I)
3350 Y=INT(Y+.5)
3360 Y=Y*(1+F9)*(-D)
3370 IF Y>9999 THEN Y=9999
3380 V1(I)=V1(I)+Y*V2
3390 RETURN
3400 PRINT 'Titrant type : ';C
3410 IF F2=1 THEN 3440
3420 PRINT 'Stat','Titrant conc.'
3430 FOR I=1 TO N \ PRINT I,M(I-1) \ NEXT I
3440 IF P1=4 THEN 3470
3450 PRINT 'Root file name : ';F$ \ PRINT 'Run ID : ';I$
3460 RETURN
3470 PRINT 'Setpoint percent tolerance : ';E1*100
3480 RETURN
3490 REM
3500 REM INPUT SETPOINTS
3510 IF S2(0)<=0 GO TO 3750
3520 REM PRINT CURRENT
3530 DISPLAY_CLEAR \ MOVE_CURSOR(12,1)
3540 FOR I=0 TO N-1
3550 PRINT 'Stat # ';I+1;'      Setpoint pH : ';S2(I)
3560 NEXT I
3570 PRINT 'Do you wish to change these ?';
3580 INPUT X$
3590 IF X$='Y' THEN 3620
3600 IF X$='y' THEN 3620
3610 RETURN
3620 PRINT
3630 PRINT 'Stat no. ( <RETURN> to quit changes) : ';
3640 GOSUB 750
3650 I=INT(X1)
3660 IF I<=0 THEN RETURN
```

```
3670 IF I<=4 THEN 3700
3680 PRINT '1 thru 4 please!'
3690 GO TO 3630
3700 PRINT
3710 PRINT 'Stat ';I;'  Setpoint : ',S2(I-1);'   New value or <RETURN
3720 GOSUB 750
3730 IF X1>0 THEN S2(I-1)=X1
3740 GO TO 3630
3750 REM
3760 REM ALL NEW VALUES
3770 DISPLAY_CLEAR \ MOVE_CURSOR(12,1)
3780 FOR I=0 TO N-1
3790 PRINT 'Stat # ';I+1;'     Setpoint pm : ';
3800 GOSUB 750
3810 IF X1>0 GO TO 3840
3820 PRINT 'Greater than 0 please!'
3830 GO TO 3790
3840 S2(I)=X1
3850 NEXT I
3860 GO TO 3490
```